

LITHIUM PHENOLATES SOLVATED BY TETRAHYDROFURAN AND 1,2-
DIMETHOXYETHANE:
STRUCTURE DETERMINATION USING THE METHOD OF CONTINUOUS
VARIATION

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by

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The role of O-Lithiated species has a very strong precedence in literature ranging from well-known reactions like Aldol, Wittig, Brook etc. in academia to their immense uses in pharmaceutical industry. According to recent study by Pfizer, over two decades, 68% of all C-C bond-forming reactions are carbanion based and 44% of them involve enolates, the most common O-Lithiated species. However, despite their prevalence, very little is known about their structure-reactivity relationships due to a lack of understanding stemming from difficulty in characterizing aggregation states in solution. Highly symmetric aggregates coupled with a spectroscopically opaque Li-O bond make this characterization really tough. The method of continuous variation in conjunction with ^6Li NMR spectroscopy has been used to characterize lithium phenolates solvated by tetrahydrofuran (THF) and 1,2-dimethoxyethane (DME) with the intention of providing a general solution to this problem. The strategy relies on the formation of ensembles of homo- and heteroaggregated phenolates and plotting them against the mole-fraction of a particular species. In this case, its worth mentioning that phenolates stand on their merits because of their stability, availability, substrate flexibility and aggregate diversity and both the solvents THF and DME offer to examine the influence of mono- and bifunctional ligands on lithium phenolate

aggregation.

With the help of this method, a very broad range of structurally (both electronically and sterically) different phenolates has been characterized both in THF and DME. While, THF affords tetrameric, dimeric, and monomeric lithium phenolates depending on solvent and substrate concentrations and on the aryl substituents, DME offers five aggregation states ranging from monomer to pentamer, a unique diversity that presumably stems in part from its capacity to serve as either a monodentate or bidentate (chelating) ligand. The occurrence of cyclic trimers and pentameric ladders uniquely in DME suggests that chelation is mandatory. The stabilization by chelation is also supported by DFT computational studies. Not only the aggregation states, the solvation number of a particular aggregation state can also be obtained by fitting the solvent dependent equilibrium of different aggregates to free solvent concentration and this technique has been used to assign solvation numbers of different aggregates in both THF and DME.

BIOGRAPHICAL SKETCH

The author was born on November 19th, 1980 in Calcutta (now Kolkata), West Bengal, India and was raised in Kalna (a small town in Burdwan District), West Bengal, India. After finishing up the high school education from Kalna Ambika Mahishamardini High School, he moved to Kolkata to continue his Bachelors study in Chemistry at Presidency College, Kolkata. He completed his B.Sc. (with Chemistry Hons.) in 2002 and joined Indian Institute of Technology, Kanpur, India to do his Master's study. In 2004, he came to USA to join the department of Chemistry at University of Illinois at Chicago (UIC) for graduate study. In 2005, he transferred to the Department of Chemistry and Chemical Biology at Cornell University. After completing all the course requirements, he joined Professor McQuade and worked in his lab from Spring 2006 to Summer 2007. Afterthat he joined Professor David B. Collum's lab and has been working in his lab since then.

To my beloved mother and Late grandfather

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LIST OF SYMBOLS

$\chi_{\mathbf{A}}$ = the mole fraction of phenolate subunits **A**

$\chi_{\mathbf{B}}$ = the mole fraction of phenolate subunits **B**

CHAPTER 1

Lithium Phenolates Solvated by Tetrahydrofuran and 1,2-Dimethoxyethane: Structure Determination Using the Method of Continuous Variation

Abstract

The method of continuous variation in conjunction with ^6Li NMR spectroscopy was used to characterize lithium phenolates solvated by tetrahydrofuran and 1,2-dimethoxyethane. The strategy relies on the formation of ensembles of homo- and heteroaggregated phenolates. The symmetries and concentration dependencies of the heteroaggregates attest to the aggregation numbers of the homoaggregates. The structurally diverse phenols afford substrate- and solvent-dependent combinations of lithium phenolate monomers, dimers, trimers, tetramers, and pentamers. We discuss the refinement of protocols for characterizing O-lithiated species. Computational studies examine further the substituent and solvent dependencies of aggregation.

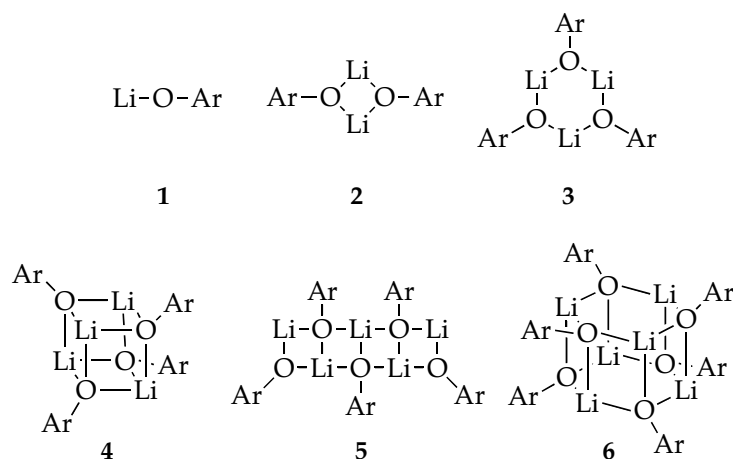
Introduction

Characterizing O-lithiated species in solution is particularly important because of their role in organic chemistry,¹ but it is a daunting task.^{2,3,4,5,6,7} Problems stem from a combination of both the high inherent symmetry of the possible aggregates and the absence of measurable Li-X scalar couplings that have in other studies proven indispensable for characterizing alkyllithiums⁸ and lithium amides.⁹ As a result, methods of characterization are indirect and often specific to the salt/solvent combination.

We have recently found the method of continuous variation^{10,11} to be a powerful and widely applicable method for characterizing lithium enolates.^{6,7} The

strategy finds its origins in studies by Chabanel,¹² Gagne,¹³ Günther,¹⁴ and others.¹⁵ We have now extended these studies to include a broad range of lithium phenolates (ArOLi) solvated by two commonly used ethereal solvents, tetrahydrofuran (THF) and 1,2-dimethoxyethane (DME). It is tempting to underscore the importance of alkali metal phenolates in the synthesis of pharmaceutical agents,¹⁶⁻¹⁸ but that would be misleading because only the more reactive sodium and potassium phenolates are prominent.¹⁹ In reality, we followed the lead of Jackman and coworkers⁵ and turned to lithium phenolates as proxies for lithium enolates.²⁰ Lithium phenolates offer desirable stability as well as considerable substrate diversity that allow for a systematic study of substrate-dependent structures. An unanticipated benefit of using lithium phenolates is the remarkable substrate-dependent array of monomers, dimers, trimers, tetramers, and pentamers (Chart 1.1, **1-5**). (Hexamers (**6**) are noticeably absent.)^{21,22,23} Such structural diversity and complexity offer opportunities for refining and stress-testing experimental protocols.

Chart 1.1. Different aggregation states of lithium phenolates observed in different solvents



This thesis follows two distinct themes. The results section describes strategies and tactics—a road map of sorts—for readers who wish to understand how the structures are assigned. The discussion section focuses primarily on the principles of solvation and aggregation.

Results

Table 1.1 summarizes the lithium phenolates studied and their resulting aggregation states and affiliated ^6Li chemical shifts. In lieu of a detailed description of each substrate-solvent combination, we summarize the types of experiments used to ascertain structure. Details are archived in APPENDIX 1. A later section illustrates how these methods can be amalgamated to assign structures to components of complex mixtures of homoaggregated phenolates.

Table 1.1. ^6Li NMR chemical shifts^a and aggregation numbers of lithium phenolates in THF/toluene and DME/toluene

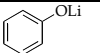
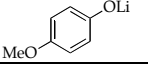
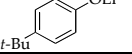
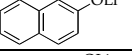
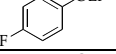
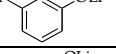
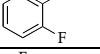
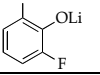
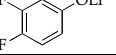
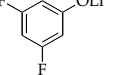
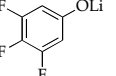
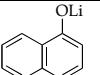
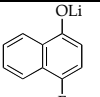
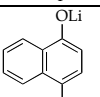
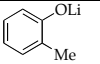
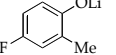
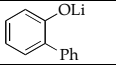
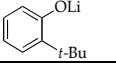
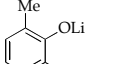
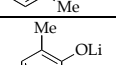
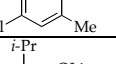
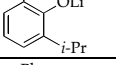
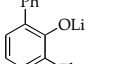
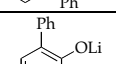
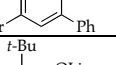
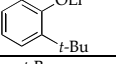
Phenolate	#	THF ^b ($\delta^6\text{Li}$)		DME ^c ($\delta^6\text{Li}$)				
		A ₂	A ₄	A ₂	A ₃	A ₄	A ₅	
	7		0.75			0.49	0.63 ^d	
	8		0.72			0.50	0.54 ^d	
	9		0.68			0.48	0.64 ^d	
	10		1.03			0.66	0.80 ^d	
	11		0.47			0.27	0.31 ^d	
	12		0.51			0.21	0.32 ^d	
	13		0.74	0.64		0.49		
	14		0.76	0.56				
	15		0.20	0.25	0.13	0.03	^e	
	16	0.15 ^f		0.19			^e	
	17	0.01 ^f		-0.02			^e	
	18	0.94 ^g	1.69	1.01	0.55			
	19	0.82 ^g	1.44 ^h	0.87	0.39			
	20	0.87 ^g	1.42	0.81	0.25			
	21	-- ⁱ	-- ⁱ	0.50	0.27			
	22	-- ⁱ	-- ⁱ	0.36	0.08			

Table 1.1. (continued)

Phenolate	#	THF ^b ($\delta^b\text{Li}$)		DME ^c ($\delta^b\text{Li}$)	
		A ₁	A ₂	A ₁	A ₂
	23		-0.21 ^j		0.08
	24		-0.12		0.26
	25		0.15 ^k		0.34
	26		-0.12 ^k		0.14
	27		0.01		0.03
	28		-0.35		-0.72
	29		-0.58		-0.97
	30	-0.02 ^g	0.63	-0.52	0.32 ^d
	31	-- ⁱ	-- ⁱ	-0.64	
	32	-0.01 ^g	0.67	-0.48	0.26 ^d

^a Chemical shifts relative to an external standard of 0.30 M ⁶LiCl in MeOH. ^b 1.2 M THF in toluene. ^c 2.9 M DME in toluene. ^d 0.22 M DME in toluene. ^e Two minor peaks, one far upfield (δ -2.6 ppm) associated with a pentamer structure inconsistent with ladder **5**. ^f 3.0 M THF in toluene. ^g Major species in neat THF. ^h Marginally soluble in 1.2 M THF/toluene. ⁱ Not characterized. ^j Major species. ^k 2.0 M THF in toluene.

Ensembles of homo- and heteroaggregates.²⁴ An ensemble of homo- and heteroaggregated phenolates (eq 1) was monitored as a function of the mole fractions of phenolate subunits (denoted generically as **A** and **B**) using ⁶Li NMR spectroscopy.^{6,7} The number of aggregates and their symmetries reflect the aggregation state, *n* (Table 1.2; Chart 1.2).¹³ Resolution of the often large number of ⁶Li resonances is maximized by pairing **A_n** and **B_n** homoaggregates with widely

separated chemical shifts. (The resonance counts for pentamers and hexamers assume slow Li-Li site exchange; vide infra.) A second parameter that influences the choice of the $\mathbf{A}_n\text{-}\mathbf{B}_n$ pair stems from the tendencies (or lack thereof) of the phenolates to form well-behaved ensembles. In short, pairs of structurally related forms (such as similarly hindered phenolates) typically provide statistical distributions⁷ that offer compelling structural assignments. To this end, pairs of phenolates differing only in the presence or absence of a para halogen proved especially useful at times.

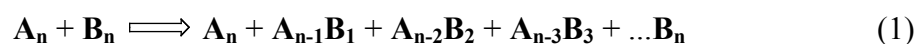


Table 1.2. Spectroscopically distinguishable aggregates in binary mixtures of lithium phenolates **A** and **B**.

aggregation

number aggregates (ratio of ⁶Li resonances)

monomer (1)	A B
dimer (2)	A₂ AB B₂
trimer (3)	A₃ A₂B (2:1)^a AB₂ (1:2)^a B₃
tetramer (4)	A₄ A₃B₁ (3:1) A₂B₂ (2:2) A₁B₃ (1:3) B₄
pentamer (5)	A₅ (2:2:1)^a A₄B₁ (3 positional isomers/13 resonances) A₃B₂ (6 positional isomers/26 resonances) A₂B₃ (6 positional isomers/26 resonances) A₁B₄ (3 positional isomers/13 resonances) B₅ (2:2:1)^a

Table 1.2. (continued)

aggregation

number aggregates (ratio of ^6Li resonances)

hexamer (6)

A_6

A_5B_1 (1:2:2:1)

A_4B_2 (3 positional isomers/9 resonances)

A_3B_3 (3 positional isomers/12 resonances)

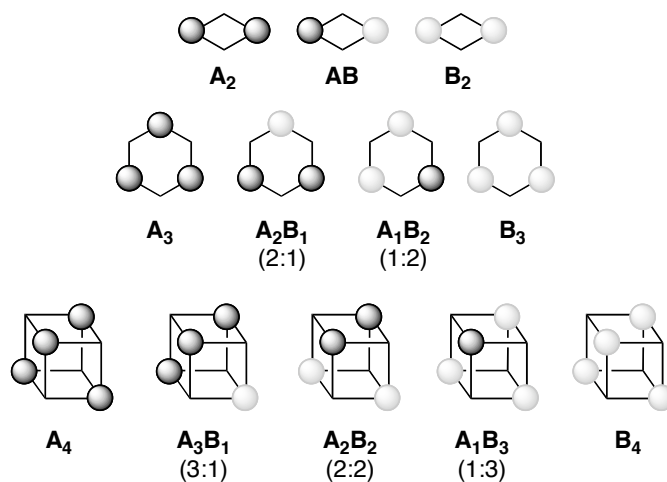
A_2B_4 (3 positional isomers/9 resonances)

A_1B_5 (1:2:2:1)

B_6

^aCounts assume a pentameric ladder in slow exchange, but the observed resonances are actually time-averaged single resonances, as described in the text.

Chart 1.2. Dimer, trimer, and tetramer mixtures showing magnetically inequivalent lithium sites.



Symmetries of homo- and heteroaggregates. ^6Li NMR spectra recorded on $\text{A}_n\text{-B}_n$ mixtures offer structural insights, as illustrated in Table 1.2 and Chart 1.2. When A_n and B_n are monomers ($n = 1$), A-B mixtures show resonances corresponding to A and B to the exclusion of additional resonances. By contrast, ^6Li spectra recorded on mixtures of A_2 and B_2 display resonances of the homodimers along with a single resonance corresponding to the AB heterodimer (Figure 1.1.a). The AB resonance is typically of intermediate chemical shift consistent with Brown's "local environment" model proffered decades ago.^{15c,25} Spectra derived from $\text{A}_4\text{-B}_4$ mixtures show single resonances for A_4 and B_4 along with 3:1, 2:2, and 1:3 resonance pairs characteristic of the A_3B_1 , A_2B_2 , and A_1B_3 heteroaggregates (Figure 1.1.b). Once again, the ^6Li chemical shifts are dominated by the proximate phenolates (local environment). Trimers are rarely observed: only in DME and invariably as components of mixtures.²⁶ Although special characterization methods required by mixtures are discussed below, a few comments about the symmetries of cyclic trimer **3** versus ladder **33** are appropriate here.²⁷ Cyclic homotrimer **3** would display a single resonance (Chart 1.2), whereas the corresponding ladder **33** would display a 2:1 pair of resonances *provided that the exchange of lithium nuclei within the aggregates—so-called intraaggregate exchange—is slow*.²⁸ In theory, A_2B_1 and A_1B_2 cyclic trimers would appear as two pairs of 2:1 resonances (four total), whereas ladder forms of A_2B_1 and A_1B_2 would afford, by virtue of positional isomerism (depicted below), as many as *ten* distinct resonances. In practice, single resonances observed for A_3 and B_3 homoaggregated trimers seem to implicate the cyclic trimer **3** motif. (Cyclic trimer derived from **19** appears as a single sharp resonance even when higher resolution ^{19}F NMR spectroscopy is used.) A_2B_1 and A_1B_2 heterotrimers, however, also appear as single, sharp resonances, indicating that intraaggregate exchange is rapid on ^6Li NMR time scales.²⁸ The high fluxionality, previously noted in DME-solvated lithium enolates,⁷

is attributed to hemilability of DME as posited in Scheme 1.1. Thus, the cyclic and ladder motifs for trimers are indistinguishable by the apparent symmetry.

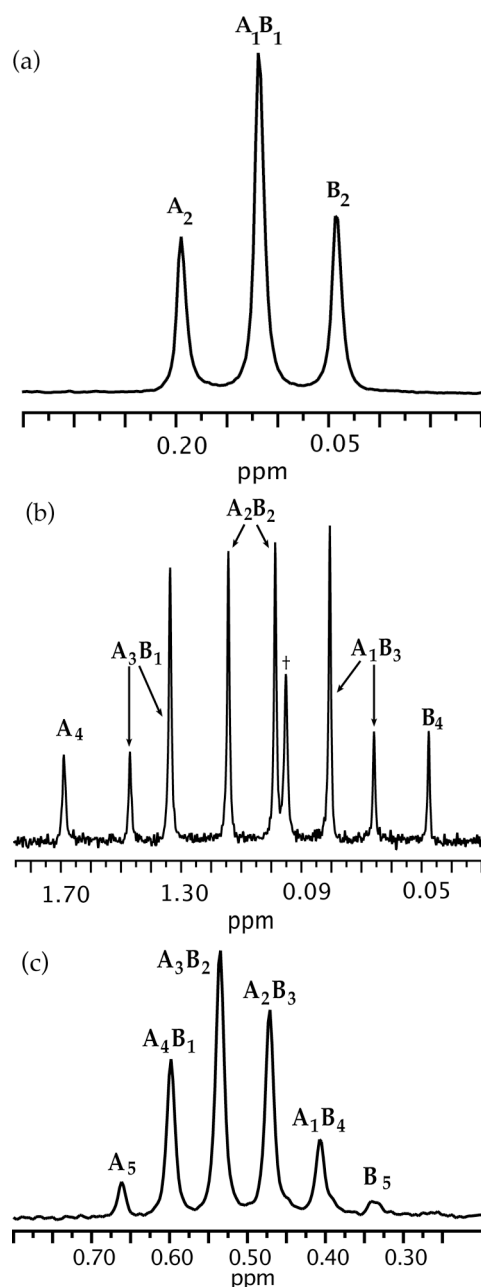


Figure 1.1. ^6Li NMR spectra recorded at -90°C of toluene solutions containing approximate 1:1 mixtures of: (a) $[\text{Li}]25$ (A) and $[\text{Li}]26$ (B) in 2.0 M THF; (b) $[\text{Li}]18$ (A) and $[\text{Li}]11$ (B) in 1.20 M THF; (c) $[\text{Li}]9$ (A) and $[\text{Li}]11$ (B) in 0.22 M DME recorded at -30°C . \dagger denotes LiHMDS dimer.

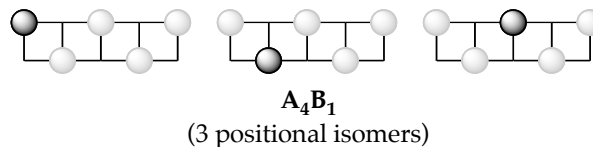
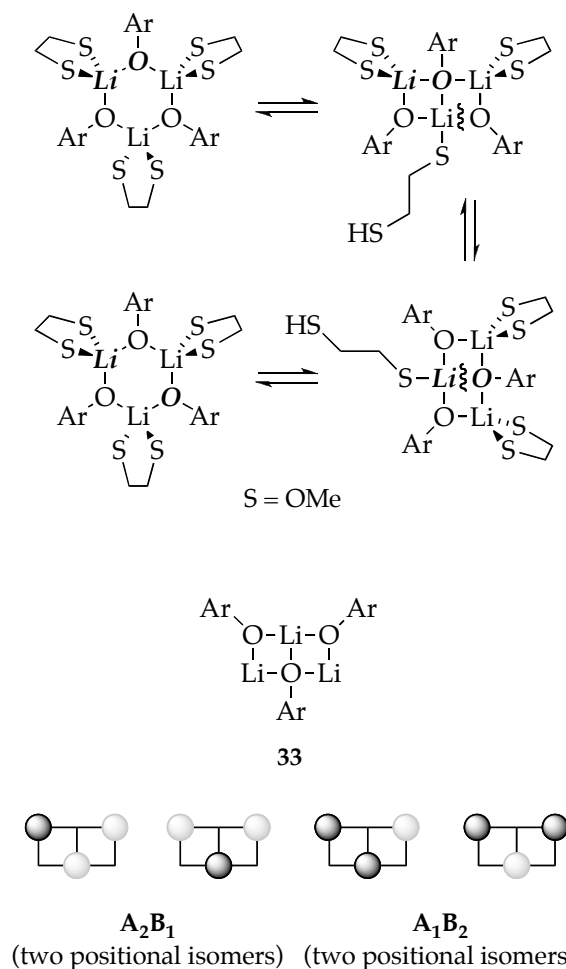


Figure 1.2. Positional isomers for ladder pentamer

Pentamers are prevalent only at low DME concentrations (<2 equiv/Li). Homoaggregated ladder **5**,^{27,29} the only pentameric form we considered seriously, should appear as a 2:2:1 triad of resonances. In practice, however, pentamers appear as very broad downfield ^6Li resonances at $-90\text{ }^\circ\text{C}$ that sharpen to single resonances and shift markedly upfield when the probe is warmed to $> -50\text{ }^\circ\text{C}$. The broadness appears to derive from partially decoalesced intraaggregate exchange, and the temperature-dependent chemical shift may result from changing solvation numbers (vide infra). Poor solubilities at low DME concentrations precluded using the lower probe temperatures required to observe pentamers by ^6Li NMR spectroscopy in the slow exchange limit. Fortunately, ^{19}F NMR spectra of fluorinated phenolates **11** and **12** revealed a well-resolved 2:2:1 triad in each case. Pentamer-derived Job plots (vide infra) are also compelling.

Ensembles of pentamers derived from A_5 - B_5 mixtures could have posed serious problems because positional isomerism (illustrated emblematically for the A_4B_1 form below) would afford 84 magnetically inequivalent ^6Li nuclei in an A_5B_5 ensemble. Indeed, spectra recorded at the lowest attainable temperatures are useless. Warming the probe above $-50\text{ }^\circ\text{C}$, however, elicits rapid intraaggregate exchange,²⁸ causing the six stoichiometrically distinct A_nB_{5-n} pentamers to appear as six well-resolved resonances (Figure 1.1.c). This exchange removes the inherent asymmetry of the ladders and the problems created by positional isomerism.⁶

Scheme 1.1. Proposed mechanism for intra-aggregate exchange of phenolate trimer in DME



Method of continuous variation.¹¹ Plots of aggregate concentrations versus mole fractions of subunits **A** and **B**—so-called Job plots¹⁰—representing the five observed aggregation states (monomers through pentamers) are illustrated in Figures 1.2-1.6. The parametric fits show that all are nearly statistical distributions; non-statistical ensembles usually attest to deep-seated structural anomalies (vide infra). The math underlying the parametric fits has been discussed previously.^{6,7}

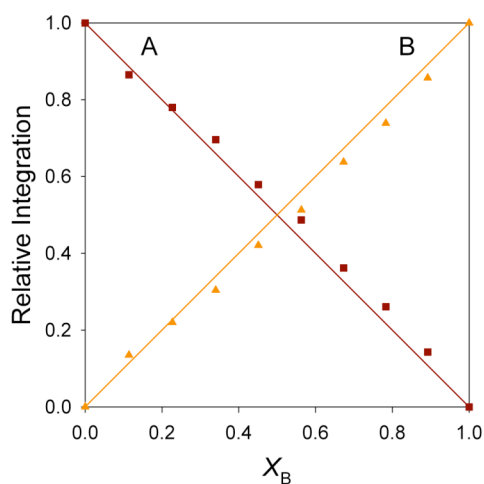


Figure 1.3. Job plot showing the relative integrations versus intended mole fractions of **31** (X_B) for 0.10 M mixtures of phenolates [^6Li]**30** (**A**) and [^6Li]**31** (**B**) in 2.9 M DME/toluene at -90 °C.

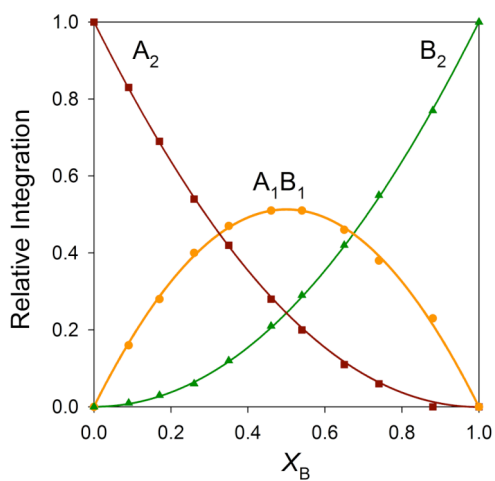


Figure 1.4. Job plot showing the relative integrations versus measured mole fractions of **29** (X_B) for 0.10 M mixtures of phenolates [^6Li]**28** (**A**) and [^6Li]**29** (**B**) in 1.2 M THF/toluene at -90 °C.

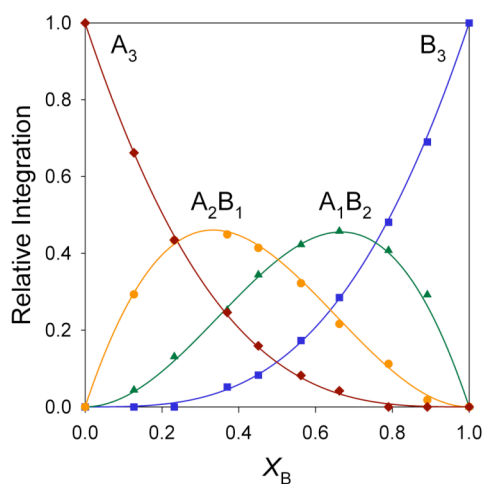


Figure 1.5. Job plot showing the relative integrations versus measured mole fractions of **20** (X_B) for 0.10 M mixtures of phenolates $[^6\text{Li}]\mathbf{18}$ (**A**) and $[^6\text{Li}]\mathbf{20}$ (**B**) in 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$

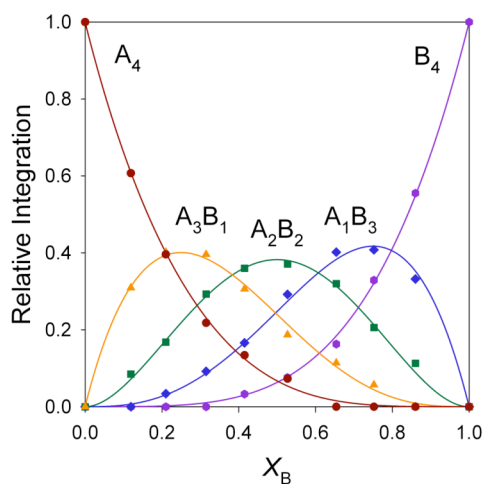


Figure 1.6. Job plot showing the relative integrations versus measured mole fractions of **11** (X_B) for 0.10 M mixtures of phenolates $[^6\text{Li}]\mathbf{9}$ (**A**) and $[^6\text{Li}]\mathbf{11}$ (**B**) in 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$.

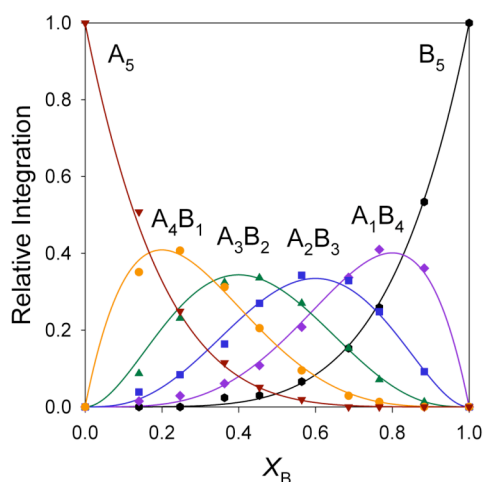


Figure 1.7. Job plot showing the relative integrations versus measured mole fractions of **11** (X_B) for 0.10 M mixtures of phenolates [^6Li]**9** (**A**) and [^6Li]**11** (**B**) in 0.22 M DME/toluene at $-30\text{ }^\circ\text{C}$.

The protocols used to measure aggregate concentrations for the Job plots require comment. The actual mole fractions of the **A** and **B** subunits can deviate from the intended mole fractions because of experimental error, nonquantitative lithiation, impurities, selective formation of mixed aggregates²⁴ with base (especially in DME),^{30,31} formation of by-products, or multiple homoaggregates (vide infra). (Some of these deviations are, admittedly, unlikely with lithium phenolates.) Although such deviations do not impair the qualitative analysis of aggregate numbers and their symmetries, they certainly distort (sometimes profoundly) the concentrations of the available **A** and **B** subunits from the intended concentrations. Consequently, the mole fractions of the **A** and **B** subunits were measured (rather than inferred from the concentrations of added phenols) by integrating the ^6Li resonances within an ensemble. Even in the cleanest and simplest cases wherein the intended and the measured mole fractions are comparable, we believe the latter to be more accurate. Job plots for monomers, however, must use the intended mole fraction because the measured mole fraction would necessarily afford perfect lines (no scatter).

Deviations from statistical behavior. Deviations from statistical behavior can occur for a variety of reasons. For example, a mixture of **25** and **27** in DME affords a single new resonance consistent with formation of a heterodimer, but with a nonstatistical (unusually high) preference. We suspect that heteroaggregation is promoted by severe steric interactions in the homodimer of **27**.^{7,32} *When distributions deviate significantly from statistical predictions, pairing substrates that are similar is constructive.* Indeed, mixtures of **25** and **26**, differing only in the absence or presence of a halogen moiety in the para position, afford statistical distributions.³³

One also observes homoaggregates that resist heteroaggregation. The obvious case occurs when two monomers are paired (**30** and **31**, for example). In a more instructive example, mixtures of **11** and **14** in DME show only traces of a new species assigned by symmetry as a heterodimer. Pairing **7** and **11** shows that **11** is tetrameric (a statistical ensemble), whereas pairing **14** and **24** reveals **14** to be dimeric. *Thus, heteroaggregation is precluded when the homoaggregates are of two different aggregation states.* In the most potentially deceptive case, a mixture of tetrameric **9** and dimeric **16** in 2.9 M DME afforded an ensemble that could easily be confused with an all-dimer **A₂-AB-B₂** ensemble. The tetramer assignment of **9** was made using independent pairings and solvent swaps (vide infra).

The most striking and provocative deviations from statistical behavior center around DME-solvated dimers. Pairing 2,6-diphenyl-substituted phenolate **28** with isostructural 4-bromo analog **29** affords a statistical **A₂-AB-B₂** ensemble; phenolate **28** in DME is clearly a dimer. Nonetheless, **28** fails to heterodimerize with seemingly similar dimeric phenolates **25** or **27**, suggesting fundamental structural differences (vide infra). Similarly, dimeric **16** and other polyhalogenated phenolates do not statistically heterodimerize with seemingly analogous dimeric hindered phenolates

(such as **27**) or orthophenylated lithium phenolate **28**. There appear to be *three types of dimers*; these are discussed further below.

Solvent swapping. A simple protocol can be used to show whether a change in solvent is accompanied by a change in aggregation.^{7,34} This protocol serves as a control experiment to confirm conclusions suggested by other data and can provide structural assignments to even minor components of mixtures.

The experiment is based on the observation that solvent-solvent exchanges (ligand substitutions) occur much faster than aggregate-aggregate exchanges.³⁵ By recording a series of spectra in which one coordinating solvent is incrementally replaced (swapped) by a second, either of two limiting behaviors can be observed: (1) If the observable forms in the two coordinating solvents differ only by ligating solvent, the incremental solvent swap will cause the resonances to exchange by time-averaging (Figure 1.8.a); (2) if the observable forms in the two solvents differ by aggregation number, an incremental solvent swap causes one aggregate to disappear and the other to appear (Figure 1.8.b). The experiment requires a ⁶Li chemical shift difference in the two solvents of as little as 0.05 ppm. Experimental data are illustrated with DME- and THF-solvated dimers of **23** (Figure 1.9) and with a DME-solvated dimer and THF-solvated tetramer of **14** (Figure 1.10).³⁶

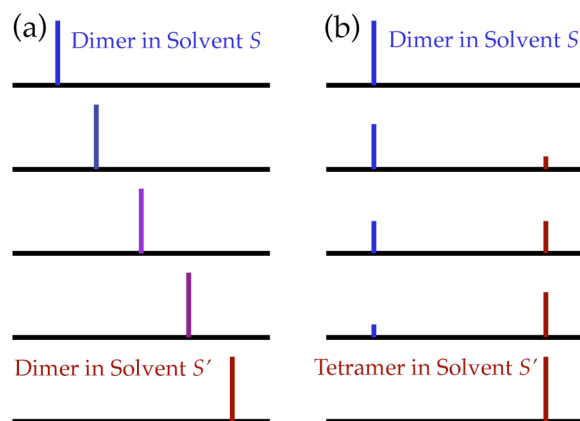


Figure 1.8. ^6Li NMR spectra anticipated if replacing solvent S by S' causes: (a) only exchange of solvent on a common phenolate aggregate (\mathbf{A}_n), and (b) an aggregation change (\mathbf{A}_m for \mathbf{A}_n).

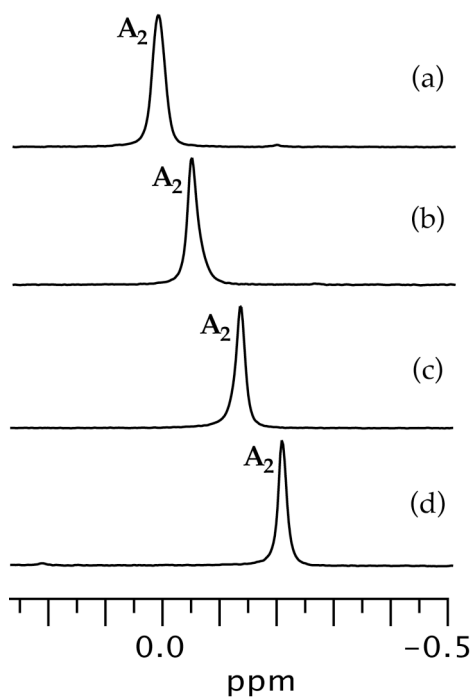


Figure 1.9. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{23}$ (\mathbf{A}) at $-90\text{ }^\circ\text{C}$ in ligand/toluene showing ligands in the following proportions: (a) 100% DME; (b) 5% THF, 95% DME; (c) 28% THF, 72% DME; (d) 100% THF.

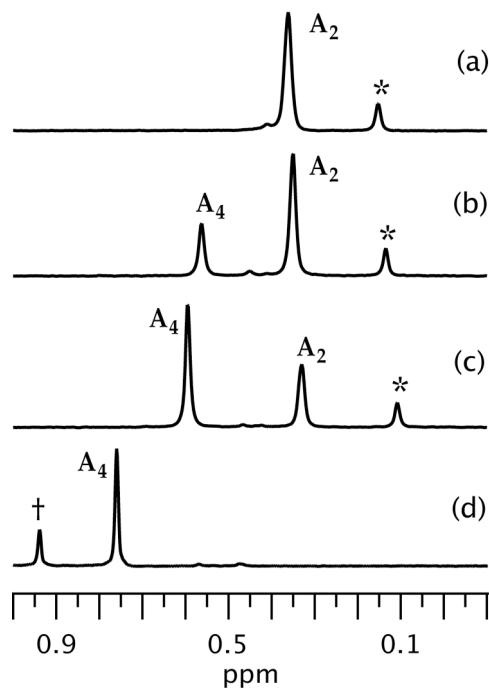


Figure 1.10. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{14}$ (**A**) at $-90\text{ }^\circ\text{C}$ in ligand/toluene showing ligands in the following proportions: (a) 100% DME; (b) 7% THF, 93% DME; (c) 16% THF, 84% DME; (d) 100% THF. * denotes $\mathbf{A}\cdot\text{LiHMDS}$ mixed aggregate; † denotes excess LiHMDS.

Phenolate concentration dependencies. To the extent that an $\mathbf{A}_n\text{-B}_n$ ensemble represents a single aggregation number (all tetramers, for example), serial dilution should confirm that the proportions of aggregates within the ensemble remain unchanged. In practice, we find that the concentration range needed to provide compelling affirmation of the assignment presents technical challenges. We carry out such control experiments but consider them of minor importance relative to more compelling data supporting aggregation state assignments. Concentration changes can, however, uncover and offer insights into homoaggregate mixtures.

Multiple aggregation states. Varying the absolute lithium phenolate concentration or, more consequential, the donor solvent concentration often reveals additional homoaggregates and their *relative* solvation and aggregation numbers. Full

characterization of such mixtures usually requires a combination of methods. Both qualitative and quantitative concentration dependencies are discussed in the next section. First, we describe Job plots on mixtures of homoaggregates.

Mixing a previously characterized aggregate such as an A_2 dimer with a B_m-B_n binary mixture in which one of the homoaggregates is a dimer typically affords a statistical A_2-AB-B_2 ensemble with one homoaggregate, leaving the other homoaggregate untouched. The success of the Job plot does not demand structural homogeneity. In some instances, mixing an A_m-A_n binary mixture with an analogous B_m-B_n binary mixture affords independent A_m-B_m and A_n-B_n ensembles (Figure 1.11). Such multiple ensembles can be engineered by pairing structurally similar phenolates, especially those differing only in the absence or presence of a para halogen substituent.

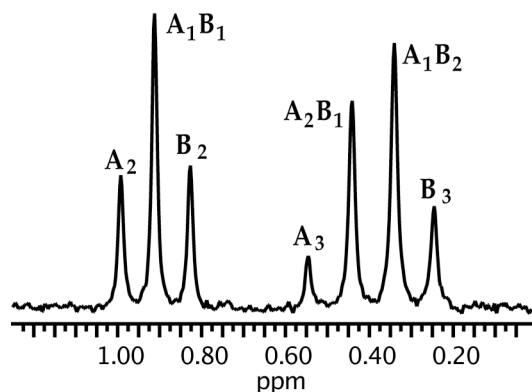


Figure 1.11. ^6Li NMR spectrum of an approximate 1:1 mixture of $[^6\text{Li}]18$ (**A**) and $[^6\text{Li}]20$ (**B**) in 2.9 M DME/toluene at -90°C .

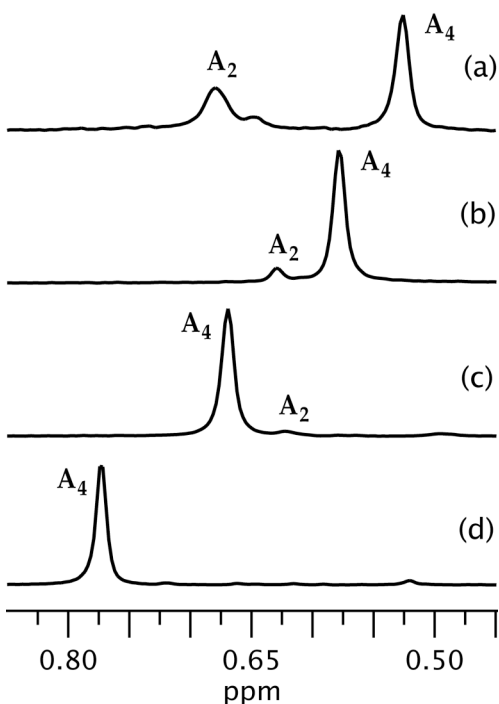


Figure 1.12. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{13}$ (**A**) at $-90\text{ }^\circ\text{C}$ in ligand/toluene showing ligands in the following proportions: (a) 100% DME; (b) 5% THF, 95% DME; (c) 16% THF, 84% DME; (d) 100% THF. * denotes $\mathbf{A}\cdot\text{LiHMDS}$ mixed aggregate.

The power of solvent swapping becomes evident when deconvoluting mixtures of homoaggregates. Combining a tetramer-dimer mixture of **13** with dimeric **27** in DME, for example, affords a statistical dimer-based ensemble, leaving the second aggregate of **13** (suspected to be tetramer) isolated. Swapping DME for THF (Figure 1.12) in the tetramer-dimer mixture of **13** shows that the putative tetramer time-averages with the fully characterized THF-solvated tetramer. Solvent swapping can even be used to identify individual components of ternary mixtures of homoaggregates.³⁷

Solvent concentration dependencies and solvation numbers. The crystallographic literature of lithium enolates and phenolates is replete with tetrasolvated tetramers.^{5,21} If one is willing to use these as benchmarks (which we are), quantitative monitoring of tetramer-dimer ratio versus THF concentration can reveal the solvation number of the dimers. Results using lithium phenolate **18** (Figure 1.13; eq 2) show that the dimers are tetrasolvated.

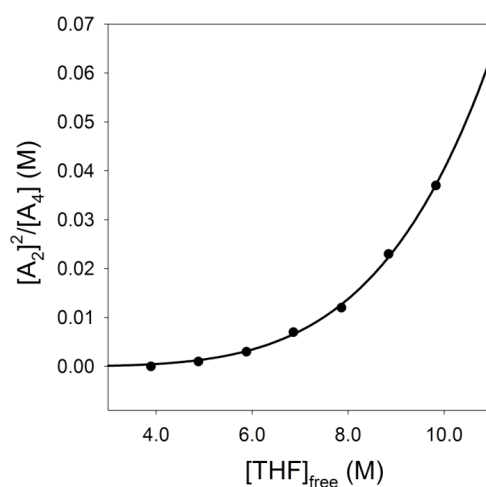


Figure 1.13. Plot of $[A_2]^2/[A_4]$ versus $[THF]_{free}$ in toluene as cosolvent for 0.11 M of phenolate **18** (**A**) at -90 °C. The curve and data represent a best-fit to the model $A_4(THF)_4 + 2n THF \rightleftharpoons 2A_2(THF)_{(n+2)}$ where $n = 2.4 \pm 0.03$.



THF-solvated monomers are only observed using acutely hindered lithium phenolates **30** and **32**. The extreme steric demand attenuates the importance of the studies because (a) the substrates are not emblematic of normal phenolates, and (b) the solvation numbers of the dimer to which the monomer assignments are anchored are not firmly established. With that said, the solvation numbers are remarkably high. Varying the THF concentrations in solutions containing monomers and dimers of **32**

reveals 3.0 additional THF ligands per lithium on the monomer relative to the dimer (Figure 1.14), which implicates tetra- or pentasolvated monomers, depending on the solvation number of the dimer (eqs 3 and 4). We know that the dimer contains at least one solvent because of a marked shift that occurs when low concentrations of THF are added to toluene solutions of **30**.

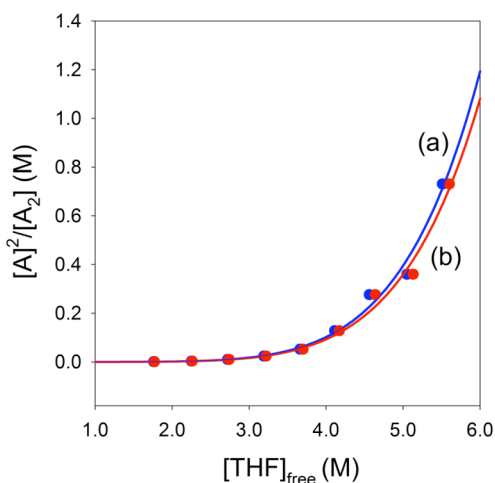
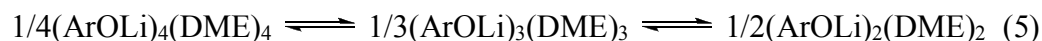


Figure 1.14. Plot of $[A]^2/[A_2]$ versus $[THF]_{free}$ in toluene as cosolvent for 0.11 M of phenolate **32** (A) at -90 °C. (a) The blue curve represents a non-linear least squares fit of the data (●) to the model $A_2 \cdot THF_4 + 2n THF \rightleftharpoons 2A_1 THF_{(n+2)}$ where $n = 3.0 \pm 0.08$. (b) The red line represents a non-linear least squares fit of the data (●) to the model $A_2(THF)_2 + 2n THF \rightleftharpoons 2A_1 THF_{(n+1)}$ where $n = 3.0 \pm 0.09$.



Varying the DME concentrations in solutions of structurally diverse DME solvates offers insights and surprises. DME-concentration-independent dimers, trimers, and tetramers attest to one solvent per lithium (eq 5).



Solvation numbers for DME-solvated monomers are assigned by monitoring the dimer-monomer ratio of phenolate **32**. Once again, measured solvation numbers are remarkably high, but the results are also somewhat quirky. Varying the DME concentrations shows that the monomer of **32** differs from the dimer by having 1.5 additional DME ligands per lithium on the monomer relative to the dimer. We know that the dimer is solvated by DME because of a marked shift that occurs when low concentrations of DME are added to toluene solutions of **32**. If this dimer is monosolvated—a structural motif that could result from severe buttressing—then the monomer is a disolvate (eq 6).³⁸ If the dimer is a disolvate, then the monomer solvation number is suggested to be 2.5 (eq 7). Such a fractional solvent order could stem from experimental error or a mixture of solvated forms. High solvation numbers are considered in the discussion.



The preference for DME-solvated pentamers only at very low DME concentrations attests to a low per-lithium solvation number, quite logically containing two DME ligands capping the ladder ends as chelates (see below). A significant (≈ 0.3 ppm) upfield shift of the time-averaged pentamer resonance with increasing temperature, however, suggests facile desolvation³⁹ of at least one internal lithium. Solvent concentration dependencies of pentamer-tetramer mixtures of phenolate **8** at -30 °C are quantitatively consistent with pentamers containing an average of three DME ligands (eq 8). The concentration dependencies suggest that tetrasolvation at

low temperature (-90 °C) is giving way to trisolvation on warming. Computations proved both supportive and instructive (vide infra).



Density functional theory computations. Computational studies of lithium enolates, phenolates, and simple alkoxides have been reported.^{40,41} We have carried out additional density functional theory (DFT) computations at the B3LYP/6-31G(d) level⁴² addressing issues of particular interest to the structural studies described herein. Me₂O was used as a model for both THF and h¹-DME to reduce the degrees of freedom. Free energies (ΔG) are reported on a *per-lithium basis* in kcal/mol at -90 °C. The results for the generic deaggregations in Scheme 2 are listed in Table 1.3. The solvation numbers and importance of chelation are consistent with the computational data archived in supporting information and seem to match experiment reasonably well. We largely refrain from detailed discussions of the absolute free energies (ΔG_1 - ΔG_6), instead focusing on the influence of substituents and solvents (trends). The substituent dependencies of ΔG_1 - ΔG_6 in Table 1.3 are considered in the discussion.

Scheme 1.2. Equilibria among different aggregation states in DME and Me₂O

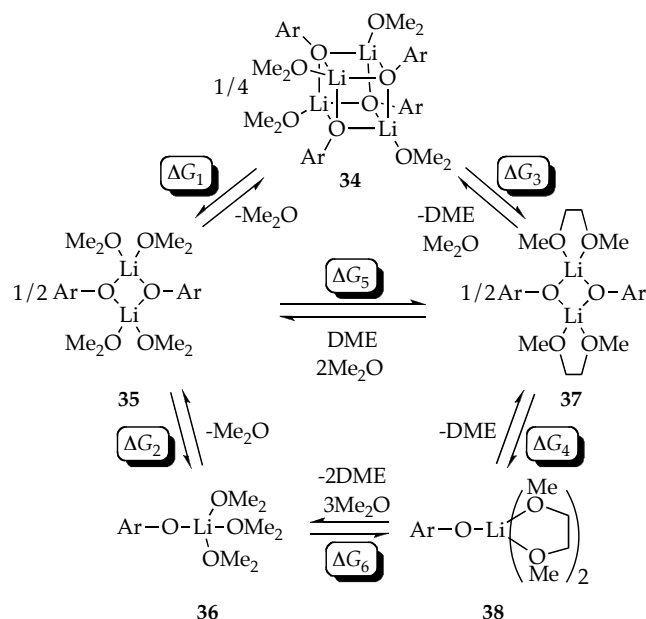
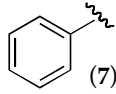
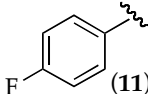
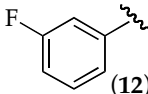
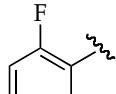
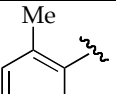
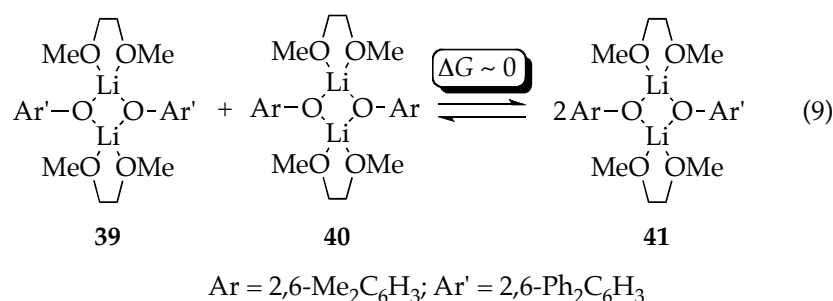


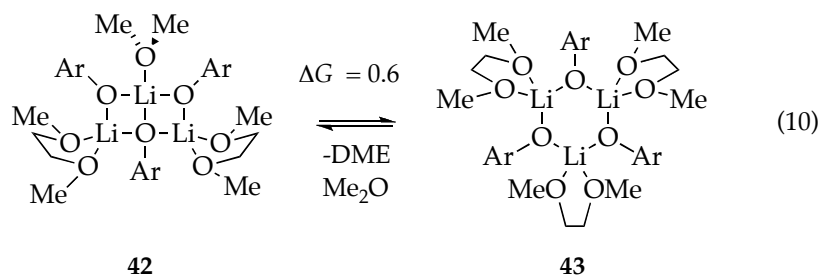
Table 1.3. Free energies ΔG_1 - ΔG_6 reported in kcal/mol on a per-lithium basis. The signs correspond to the affiliated arrows in Scheme 1.2.

-Ar (#)	ΔG_1	ΔG_2	ΔG_3	ΔG_4	ΔG_5	ΔG_6
 (7)	3.67	10.43	-0.11	10.05	-3.78	-4.16
 (11)	3.79	9.86	-0.14	10.23	-3.92	-4.29
 (12)	3.27	10.59	-0.03	8.98	-3.30	-4.91
 (13)	3.80	9.25	-0.36	7.21	-3.47	-5.51
 (25)	0.21	6.75	-6.22	10.06	-6.40	-3.12

We experimentally detected what appears to be three classes of lithium phenolate manifesting (1) intermediate sterics demands, (2) high electron deficiency (polyfluorination), and (3) 2,6-diphenylation. Experimentally, dimmers within one class afford decidedly nonstatistical heterodimer ensembles with phenolates from another class. We examined this finding computationally using lithium phenolates **25** and **28** (eq. 9). In short, the computations showed no significant deviations of the homodimer-heterodimer equilibrium from statistical, underscoring an uncontested agreement between theory and experiment. In this context, we re-evaluated the experimental data and stand behind it.

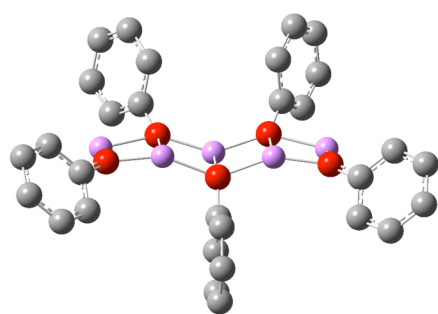


Cursory computational studies of the rarely observed DME-solvated trimers showed triply chelated cyclic form **43** to be more stable than ladder **42** bearing an η^1 solvate. We proffered the ladder as an intermediate in the rapid intraaggregate exchange (Scheme 1.1).

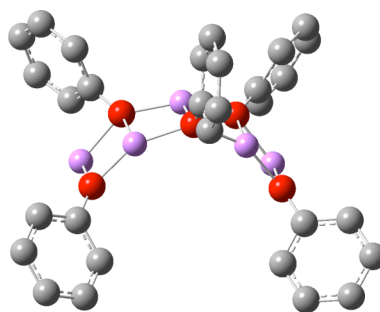


*Energy in kcal/mol on a per-lithium basis at -90 °C.

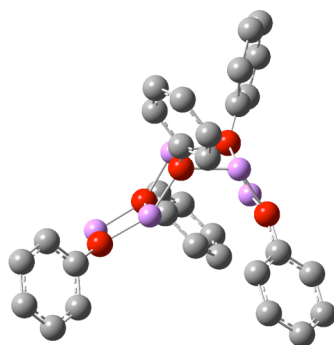
Computations evaluated the geometry and stabilities of DME-solvated pentameric ladders, suggested by experiment to be a temperature-sensitive mixture of tri- and tetrasolvates. Three geometries—W, U, and a hybrid (Figure 1.15, **44-46**)—are stable minima in their unsolvated, doubly chelated forms; the U form (**47**) is the most stable. Me₂O was used to model the solvation of the internal lithiums by monodentate (η^1) DME ligands (Scheme 3). Tetrasolvate **51** is calculated to be preferred at temperatures below -74 °C, whereas trisolvate **50** is favored above -74 °C. Thus, the computations successfully mimic the putative temperature-sensitive desolvation detected experimentally. We were also struck by the allosteric effects, phenomena we have referred to as correlated solvation.



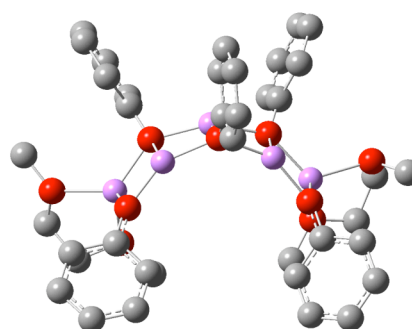
44: “W-shaped”



45: “U-shaped”



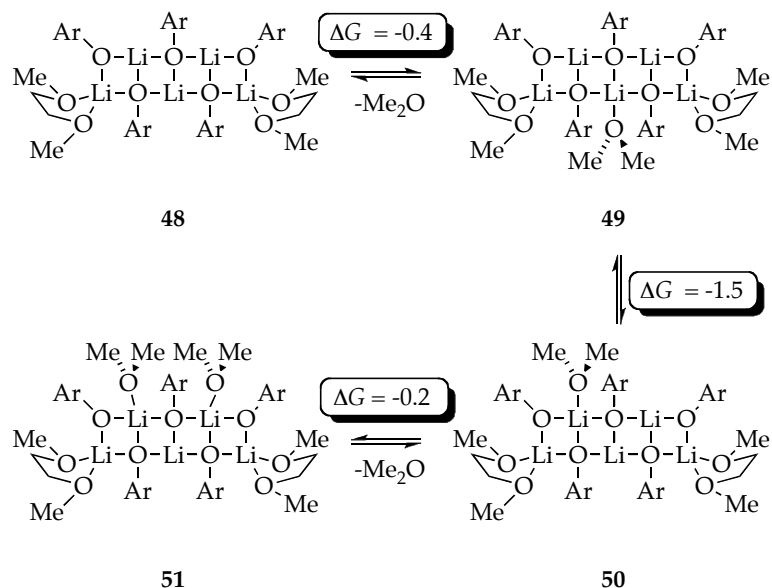
46: Hybrid



47: Disolvated “U-shaped”

Figure 1.15. Optimized structures of ladder pentamers

Scheme 1.3. Equilibria among different solvation states ladder pentamers



*All U-shaped; energies reported in kcal/mol on a per-lithium basis at -90 °C.

Discussion

Lithium salts are centrally important in such disparate fields as organic synthesis,⁴⁴ polymer science,⁴⁵ electrochemistry,⁴⁶ medicine,⁴⁷ and automotive lubricants.⁴⁸ We have been refining protocols that are based on the method of continuous variation—the method of Job—for characterizing O-lithiated species.^{10,11} Our interest in the phenolates stems from our desire to develop and refine methods for characterizing their more synthetically important lithium enolate counterparts. Nonetheless, lithium phenolates stand on their own merits because of their stability, purity, availability, substrate flexibility, and aggregate diversity. Examination of a broad array of lithium phenolates in THF and DME solutions revealed a remarkable range of aggregates from monomers through pentamers (**1-5**) and underscored the versatility of these methods.

The problems associated with characterizing LiX species in which the X group is magnetically opaque have been long-standing and acute.⁴⁹ The seemingly most

general and certainly most popular methods involve measuring colligative properties of solutions, which afford average molecular weights.^{2,4,5,19,45,49} Although colligative measurements can provide valuable supporting evidence of structure, as stand-alone methods they are fraught with risk because of problems caused by undetected impurities and mixtures of structural forms. Methods that are also germane to our tactic involve quantitatively monitoring LiX-LiY mixed aggregates constituted from the LiX salt of unknown structure and an LiY salt of known structure.^{3,12-15,50,51} In general, progress has been made—enolate studies of Streitwieser and coworkers are certainly notable³—but the strategies used are often quite specific to the LiX-solvent combination.

Of particular importance to the work described herein, Jackman and coworkers investigated the structures of lithium phenolates using a combination of methods in which ⁷Li quadrupolar splitting constants and predicted chemical shifts of ¹³C resonances derived from the para carbons were of paramount importance.⁵ Obviously their method applies only to lithium phenolates and not other O-lithiated species. They also focused on a smaller and different subset of lithium phenolates as well as a number of solvents not described herein. Their emphasis on enthalpic and entropic differences in aggregates to ascertain relative solvation numbers appears to be challenging at best. But the congruence of our results and conclusions and those of Jackman and coworkers are notable despite the use of distinctly different approaches.

Methods. Our strategy for characterizing lithium phenolates entails breaking the high inherent symmetry (spectral simplicity) of (ROLi)_n aggregates by mixing two homoaggregates (**A_n** and **B_n**) and generating ensembles containing both homo- and heteroaggregates (eq 1).^{6,7} The numbers and symmetries of the heteroaggregates, as shown by ⁶Li NMR spectroscopy, offer considerable insights into the structures of the

homoaggregates (Table 2; Chart 2). By systematically varying the mole fractions of the **A** and **B** subunits, we can use parametric fits to afford the Job plots illustrated emblematically in Figures 1.2-1.6. Statistical distributions observed for structurally similar phenolates (some varying by as little as a para halogen substituent) confirm the structural assignments, whereas marked deviations from statistical usually foreshadow different aggregation numbers for **A_m** and **B_n**. Once **A_n** is characterized in one solvent (such as DME) and an aggregate of unknown aggregation number is generated in a different solvent (THF), one can trivially ascertain if the aggregation number differs in the two solvents by a simple experiment illustrated in Figures 7-9 in which DME is incrementally replaced (swapped) by THF. Lithium phenolates distinguished only by the coordinated ligands display a single time-averaged ⁶Li resonance, whereas phenolates of differing aggregation number appear as discrete resonances.

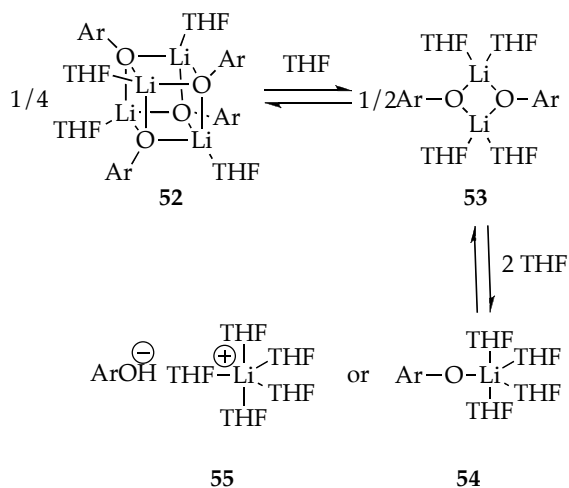
Varying the solvent and phenolate concentrations often reveals additional homoaggregates and provides qualitative insight into their relative aggregation and solvation numbers. In some instances, combining **A_m**-**A_n** mixtures with **B_m**-**B_n** mixtures afford two fully separate **A_m**-**B_m** and **A_n**-**B_n** ensembles that are easily and independently quantified. In other cases, solvent swaps reveal the structures of homoaggregates irrespective of the total number of homoaggregates. In fact, one of the more satisfying outcomes is that essentially any mixture can be characterized provided that discrete resonances are observed. One cannot, however, overstate the importance of using complementary methods as well as multiple combinations of aggregates. Overdetermination of structure is important.

Solvent effects. THF and DME were used to examine the influence of mono- and bifunctional ligands on lithium phenolate aggregation. THF affords tetrameric, dimeric, and monomeric lithium phenolates depending on solvent and substrate

concentrations and on the aryl substituents (discussed below). By contrast, DME affords five aggregation states, a diversity that may stem in part from its capacity to serve as either a monodentate or bidentate (chelating) ligand.⁵² The occurrence of cyclic trimers (**3**) and pentameric ladders (**5**) uniquely in DME suggests that chelation is mandatory. Stabilization by chelation is supported by computational studies (Scheme 2; Table 3). Qualitative data from the solvent swaps suggest that the computations may, however, overestimate the relative stability of the DME-solvated dimers (**37**).³⁶

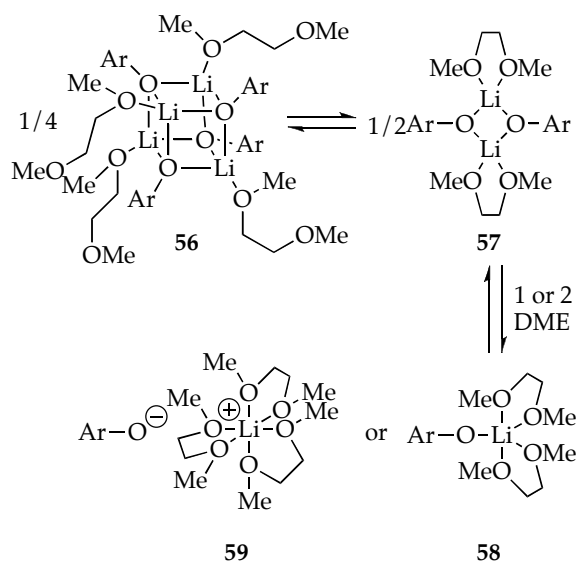
THF solvation numbers were assigned by monitoring how the tetramer, dimer, and monomer concentrations varied with THF concentration (Scheme 1.4). The tetramer and dimer numbers enjoy full computational support. The monomer solvation numbers, by contrast, are a little more difficult to interpret because only the extraordinarily hindered 2,6-di-*tert*-buyl derivatives afford monomers. Certainly phenolate **30** is not representative of phenolates in general. The data, however, support *tetra- or pentasolvates* **54** and **55**, respectively. Tetrasolvated monomer (Me₃Si)₂NLi(THF)₄,⁵⁴ as well as other evidence of high-coordinate lithium, support the tetrasolvate **54**.⁵³⁻⁵⁷ Putative pentasolvate **55** is supported by crystallographically characterized +Li(THF)₅ and +Li(THF)₆ cations.⁵⁴ Nonetheless, such high solvation numbers were unanticipated and certainly are inconsistent with conventional wisdom.

Scheme 1.4. Different equilibria among tetramer, dimer and monomeric states in THF



Analogous studies of DME-solvated aggregates afford results comparable to those found with THF (Scheme 1.5). Equivalent per-lithium solvation numbers of the tetramers (**56**) and dimers (**57**) are consistent with h^1 and h^2 -coordinated DME, respectively. The η^1 -DME ligands on **56** may seem a little odd on first inspection, but their presence is supported by analogy to crystallographic and solution structural studies of other DME-solvated organolithiums.⁵⁸ Chelation in dimer **57** has ample crystallographic and computational support, requiring little further justification.²¹

Scheme 1.5. Different equilibria among tetramer, dimer and monomeric states in DME



Once again, the monomers give us pause because of the extraordinary steric demands of phenolate **30** required to observe them. Moreover, the solvation numbers of the monomers are measured *relative* to the dimers, but we are not fully confident that such hindered dimers are doubly solvated. Consequently, doubly-chelated monomer **58** and ion-paired monomer **59** are both consistent with the data. Five-coordinate $\text{LiX}(\eta^2\text{-DME})_2$ complexes support the proposed structure of monomer **58**,^{55,56} and the well-precedented $+\text{Li}(\eta^2\text{-DME})_3$ cation supports that of **59**.⁵⁷ There is a significant argument against **59**: A mixture of putative ion pairs derived from lithium phenolates **30** and **31** show two distinct lithium cations. The origin of such a slow gegenion exchange is unclear. Regardless of the details, the high solvation numbers are surprising.

Trimers are observed only in DME, for a limited number of phenolates, and never as major components. The per-lithium solvation number of DME-solvated trimers is the same as those of dimers and tetramers (one per lithium). Rapid ^6Li

intraaggregate exchange (speculatively presented in Scheme 1) precluded distinction of a ladder versus a cyclic form of the trimers; computational studies support the cyclic form (eq 10). Based on analogy with other lithium derivatives (lithium amides in particular) in which solvated trimers appear to be sterically more problematic than their cyclic dimer counterparts, we suspect the low steric demands of DME chelates may be important.⁵⁹

The exotic and unanticipated pentameric ladders are prevalent at low DME concentrations. Rapid intraaggregate exchange obscures their asymmetry using ^6Li NMR spectroscopy, but 2:2:1 triads of resonances were observed using ^{19}F NMR spectroscopy on two fluorinated substrates. At the outset, the low per-lithium solvation number suggested that the ends of the ladders are capped by chelating DME ligands. Concentration and temperature dependencies evidence weak solvation of *one* of the internal lithiums. Computations support a ladder capped by chelating DME ligands and indicate a marked preference for U-shaped rather than W-shaped ladders (**45** and **44**, respectively). Moreover, the computations support partial solvation of the internal lithiums (Scheme 1.3). It is not obvious, however, why pentameric ladders are the only observable ladder forms (assuming, of course, that the trimers are cyclic). Although U-shaped (concave) hexameric ladders would be sterically problematic, tetrameric ladders seem plausible at low DME concentration but are not observed.⁶⁰

Electronic effects. Lithium phenolates are ideally suited for examining the influence of electronic effects on aggregation. Monohalogenated phenolates **11-13** are unperturbed enough to elicit measurable aggregation state changes. By contrast, computations of multiply halogenated phenolates **14-17** clearly show that halogens promote deaggregation (Table 1.1).⁶¹ Moreover, comparing phenolate **15** and **16** under similar conditions shows that the meta fluoro moieties promote deaggregation

more so than para moieties do. There are parallels with the pK_{As} of 3- and 4-phenols.⁶² The meta substituent and its W relationship to the anionic phenolate oxygen appears optimally oriented to influence aggregation. Computational studies comparing monofluorinated lithium phenolates with the parent phenolate **7** show that ortho>meta>para at promoting deaggregations. (Apparent Li-F contacts in THF-solvates obscure insights into the electronic effects of ortho fluoro moieties.)

Steric effects. Considerable empirical evidence suggests that high steric demands promote deaggregations of lithium salts because of the severe van der Waals interactions within the aggregates.³² Phenolates **18-32** are sterically demanding to some extent, and all show a greater penchant for forming dimers than do simple phenolates. Only the most severely congested phenolates buttressed by two *tert*-butyl groups (**30-32**) afford monomers. Computations comparing parent phenolate **7** and 2,6-dimethyl phenolate **25** (Table 1.3) confirm that congestion promotes dimers relative to tetramers and monomers relative to dimers.

Like aggregates with like. It seems self-evident—a truism—that LiX salts are most likely to modify the reactivity and selectivity of organolithium reactions if they form mixed aggregates.^{24,44} One of the most interesting and potentially important observations, therefore, is that heteroaggregation is promoted by pairing species that are similar.

A₄ and **B₄** mixtures usually afford ensembles of tetramers that are nearly statistical. The same is true for other analogous **A_n-B_n** pairs. By contrast, **A₄** tetramers and **B₂** dimers resist heteroaggregation. It seems logical in retrospect that a homoaggregate would resist heteroaggregation if it meant forfeiting a preferred aggregation number. For this reason, we place great importance on statistical

ensembles. Of course, there are exceptions. We observed that **A₄-B₂** mixtures derived from **9** and **16** (respectively) in THF afford no heterotetramers but do afford heterodimers. Homoaggregates that are on the cusp of shifting aggregation number are likely to be more promiscuous at heteroaggregation.

Not all dimers are alike. There appear to be three albeit loosely defined classes of dimers: (1) sterically congested lithium phenolates (**18-27**), (2) highly electron-deficient lithium phenolates (**14-17**), and (3) 2,6-diphenylated lithium phenolates (**28** and **29**). Pairs chosen from two different classes tend to form nonstatistical ensembles (sometimes markedly so). Classes 1 and 2 form heteroaggregates that are prone to deviate from statistical distributions in both directions. 2,6-Diphenylated substrates **28** and **29** present the most vexing category.⁶³ They seem to have steric demands akin to dimeric phenolates **25-27** and electronic properties that *could* be similar to polyfluorinated derivatives **14-17**, yet they form heterodimers only with each other, not with class 1 or 2 dimers. It was somewhat disappointing and even somewhat disconcerting that computational studies completely failed to mimic these results, affording statistical distributions for all combinations (eq 9).

Conclusions

There may be a niche market for insights into the structures of lithium phenolates. The work described herein, however, has broader implications. Characterizing lithium salts with an NMR-inactive gegenion has been a long-standing problem of considerable importance. The strategies and tactics described in this manuscript appear to offer general solutions, especially for O-lithiated species.^{6,7} It became increasingly apparent as the work progressed that the view of substrate-

dependent aggregation provided by lithium phenolates may be unique.⁵ Those interested in understanding the solution structures of lithium halides have a very limited choice.⁴⁹ Similarly, we have studied lithium amides for almost 25 years,³⁹ yet we have examined in detail less than a dozen variations of the dialkylamido moiety, which is hardly systematic. The breadth and number of alkyllithiums studied to date is impressive,⁸ but an RLi dependence is difficult to systematize. By contrast, lithium phenolates allow for a reasonably systematic study of how changing X in LiX salts influences aggregation state.

Our interest in lithium phenolates as vehicles for studying salt effects in solution has been piqued and will persist. The advantages and synergies of studying several solvents concurrently became evident in these studies and, in conjunction with Jackman's early studies,⁵ should gain momentum with each additional solvent. The low basicity of lithium phenolates should allow us to study metal ion solvation by a very broad range of solvents, including many that are incompatible with more reactive organolithium derivatives.

Experimental Section

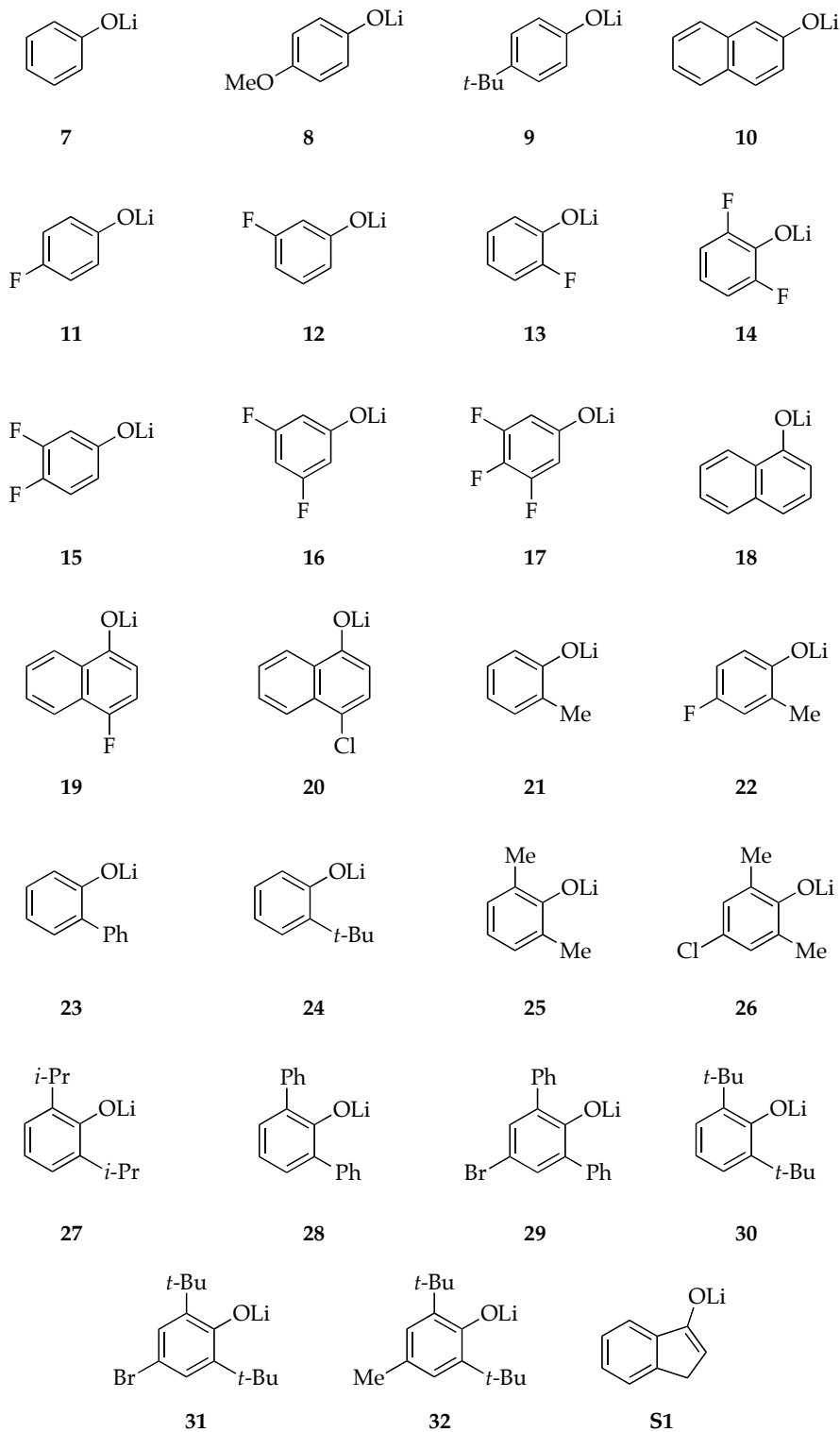
Reagents and Solvents. DME, THF, and toluene were distilled from solutions containing sodium benzophenone ketyl. The toluene stills contained approximately 1% tetraglyme to dissolve the ketyl. We prepared and recrystallized [⁶Li]LiHMDS and [⁶Li, ¹⁵N]LiHMDS as described previously.³¹ Air- and moisture-sensitive materials were manipulated under argon using standard glove box, vacuum line, and syringe techniques. The precursor to **29** was prepared using standard halogenation procedures.⁶⁴

Spectroscopic Analysis. Individual stock solutions of substrates and base were prepared at room temperature. An NMR tube under vacuum was flame dried on a Schlenk line and allowed to come to room temperature. It was then backfilled with argon and placed in a -78 °C dry ice/acetone bath. The appropriate amounts of the base and substrate were added sequentially via syringe. The tube was sealed under partial vacuum, vortexed for approximately 10 seconds at room temperature, and cooled to -78 °C. Each NMR sample contained 0.10 M total phenolate and 0.11 M LiHMDS.

^6Li NMR spectra were typically recorded at -90 °C (unless stated otherwise) on a 400 or 500 MHz spectrometer with a delay between scans set to $>5 \times T_1$ to ensure accurate integrations. Chemical shifts are reported relative to a 0.30 M $^6\text{LiCl}/\text{MeOH}$ standard at the reported probe temperature. The resonances were integrated using standard software accompanying the spectrometers. After weighted Fourier transform with 64,000 points and phasing, line broadening was set between 0 and 0.2, and a baseline correction was applied when appropriate. Deconvolution was performed in the absolute intensity mode, with application of a drift correction using default parameters for contributions from Lorentzian and Gaussian line shapes. For poorly resolved spectra, the resonances were indicated using the mark and use-mark commands. The math underlying the parametric fits has been described in detail.^{6,7a}

APPENDIX 1

Chart A1.1. Structures of phenolates and Indanone enolates



I. Combinations of O-lithiated species in THF, DME and TMEDA: Job plots.

For a full list of Job plots and their corresponding page numbers, see **Table A1.1**

II. Solvent swaps:

For a full list of solvent swaps and their corresponding page numbers, please see **Table A1.2**

III. Solvent concentration scans.

For a full list of solvent concentration scans and their corresponding page numbers, please see **Table A1.3**

IV. Phenolate concentration scans.

For a full list of phenolate concentration scans and their corresponding page numbers, please see **Table A1.4**

V. ^{19}F NMR spectra.

- | | |
|---|-----|
| a. Temperature profile of pentameric 11 in 0.22 M DME/toluene. | 138 |
| b. Dimer and trimer of 19 in 2.9 M DME/toluene. | 139 |
| c. Dimer and trimer of 22 in 2.9 M DME/toluene. | 140 |

VI. Computational Studies.

- | | |
|--|---------|
| a. Equations describing the equilibria modeled computationally. | 141-148 |
| b. For optimized geometry at B3LYP level of theory with 6-31G(d) basis set, free energy (G, Hartrees), and cartesian coordinates (X, Y, Z), please see Table A1.5 | 149-240 |

**Table A1.1. Combinations of O-lithiated species in THF, DME and TMEDA:
Job plots.**

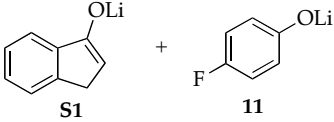
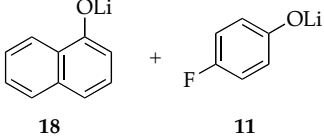
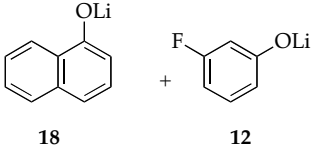
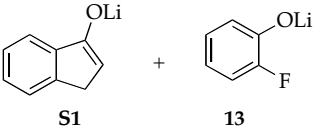
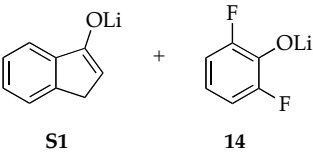
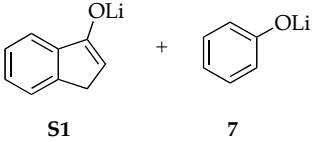
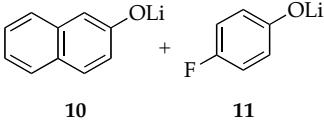
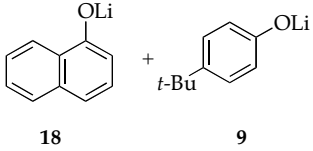
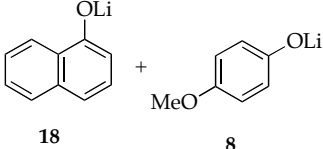
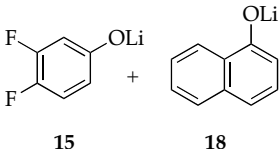
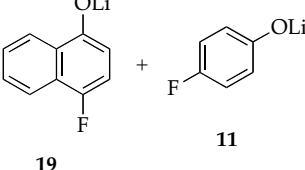
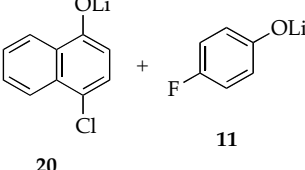
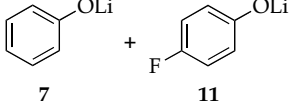
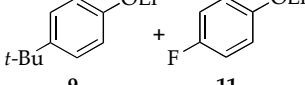
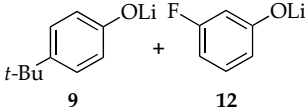
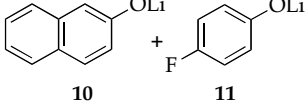
Substrate Combinations	Page	Structure (s)	Solvent
 S1 + 11	50	Tetramers	THF
 18 + 11	51	Tetramers	THF
 18 + 12	52	Tetramers	THF
 S1 + 13	53	Tetramers	THF
 S1 + 14	54	Tetramers	THF
 S1 + 7	55	Tetramers	THF
 10 + 11	56	Tetramers	THF
 18 + 9	57	Tetramers	THF

Table A1.1. (continued)

 <p>18 + 8</p>	58	Tetramers	THF
 <p>15 + 18</p>	59	Tetramers	THF
 <p>19 + 11</p>	60	Tetramers	THF
 <p>20 + 11</p>	62	Tetramers	THF
 <p>7 + 11</p>	63	Tetramers	DME
 <p>9 + 11</p>	64	Tetramers	DME
 <p>9 + 12</p>	65	Tetramers	DME
 <p>10 + 11</p>	66	Tetramers	DME

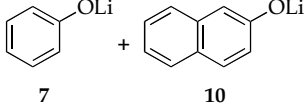
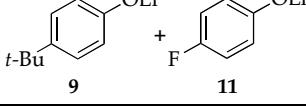
 <p>7 + 10</p>	67	Pentamers	DME
 <p>9 + 11</p>	68	Pentamers	DME

Table A1.1. (continued)

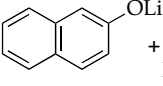
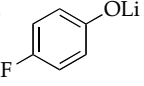
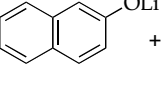
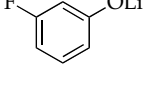
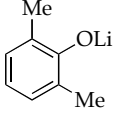
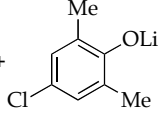
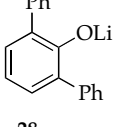
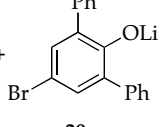
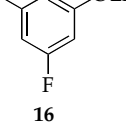
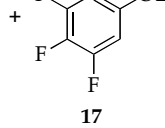
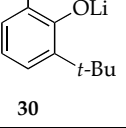
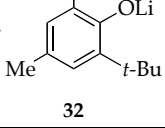
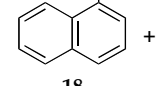
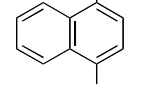
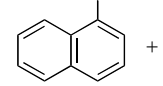
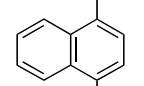
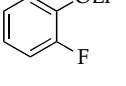
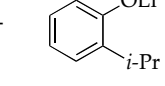
 10	 11	69	Pentamers	DME
 10	 12	70	Pentamers	DME
 25	 26	71	Dimers	THF
 28	 29	72	Dimers	THF
 16	 17	73	Dimers	THF
 30	 32	74	Dimers	THF
 18	 19	76	Dimers	THF
 18	 20	78	Dimers	THF
 13	 27	79	Dimers	DME

Table A1.1. (continued)

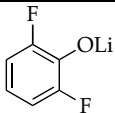
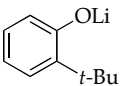
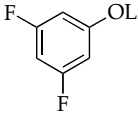
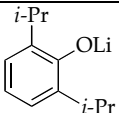
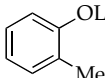
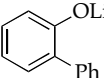
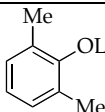
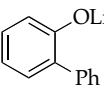
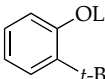
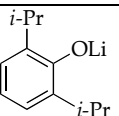
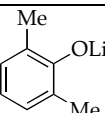
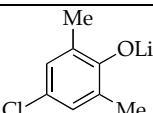
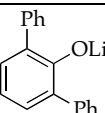
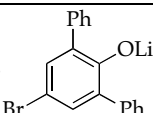
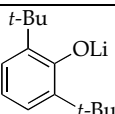
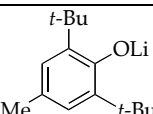
 14	+	 24	81	Dimers	DME
 16	+	 27	82	Dimers	DME
 21	+	 23	83	Dimers	DME
 25	+	 23	84	Dimers	DME
 24	+	 27	85	Dimers	DME
 25	+	 26	86	Dimers	DME
 28	+	 29	87	Dimers	DME
 30	+	 32	88	Dimers	DME

Table A1.1. (continued)

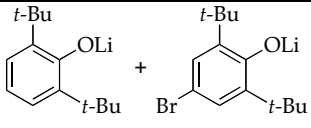
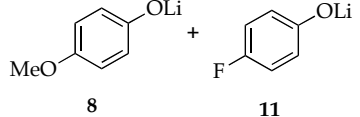
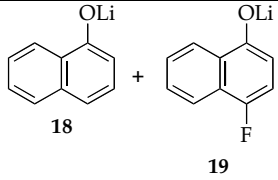
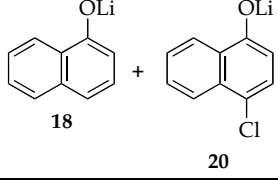
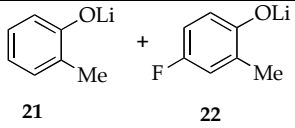
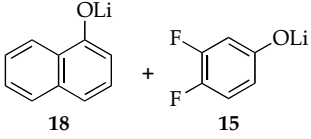
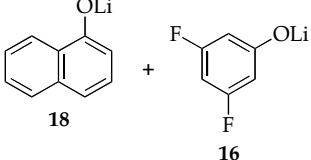
 <p>30 31</p>	89	Monomers	DME
 <p>8 11</p>	90	Pentamers Tetramers	DME
 <p>18 19</p>	91	Dimers Trimers	DME
 <p>18 20</p>	93	Dimers Trimers	DME
 <p>21 22</p>	94	Dimers Trimers	DME
 <p>18 15</p>	95	Dimers	TMEDA
 <p>18 16</p>	96	Dimers	TMEDA

Table A1.2. Solvent swaps.

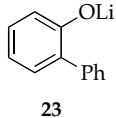
Substrate	Solvent 1	Solvent 2	Page no.
 <p>23</p>	2.9 M DME/toluene	1.1 M THF/toluene	97

Table A1.2. (continued)

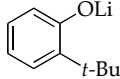
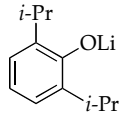
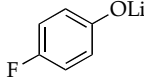
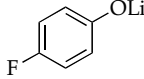
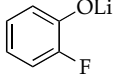
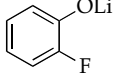
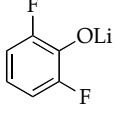
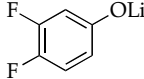
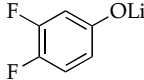
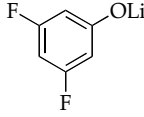
 24	2.9 M DME/toluene	1.1 M THF/toluene	98
 27	2.9 M DME/toluene	1.1 M THF/toluene	99
 11	2.9 M DME/toluene	3.7 M THF/toluene	100
 11	2.9 M DME/toluene	2.0 M TMEDA/toluene	101
 13	2.9 M DME/toluene	1.1 M THF/toluene	102
 13	2.9 M DME/toluene	0.22 M TMEDA/toluene	103
 14	2.9 M DME/toluene	1.1 M THF/toluene	104
 15	2.9 M DME/toluene	1.1 M THF/toluene	105
 15	2.9 M DME/toluene	0.22 M TMEDA/toluene	106
 16	2.9 M DME/toluene	0.18 M TMEDA/toluene	107

Table A1.2. (continued)

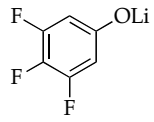
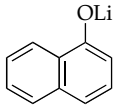
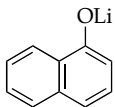
 17	2.9 M DME/toluene	3.7 M THF/toluene	108
 18	2.9 M DME/toluene	3.7 M THF/toluene	109
 18	2.9 M DME/toluene	2.0 M TMEDA/toluene	110

Table A1.3. Solvent concentration scans.

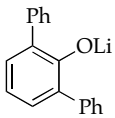
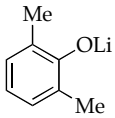
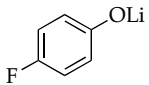
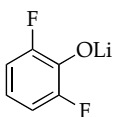
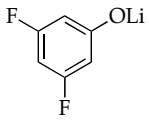
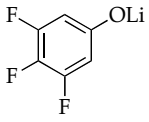
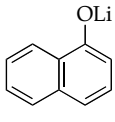
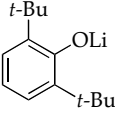
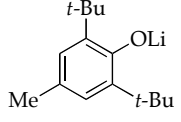
Substrate	Solvent	Lower limit	Upper limit	Page no.
 28	THF	1.2 M	12.2 M	111
 25	THF	2.0 M	10.0 M	112
 11	THF	0.12 M	12.2 M	113
 14	THF	2.0 M	10.0 M	114

Table A1.3. (continued)

 16	THF	2.0 M	10.0 M	115
 17	THF	3.0 M	8.0 M	116
 18	THF	2.0 M	12.2 M	117
 30	THF	2.0 M	10.0 M	119
 32	THF	4.0 M	12.2 M	120

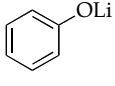
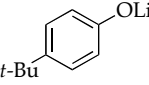
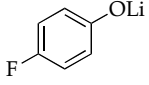
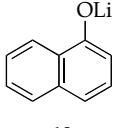
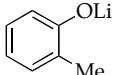
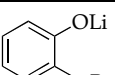
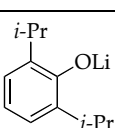
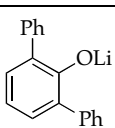
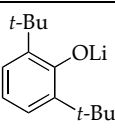
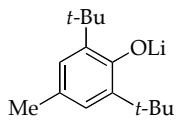
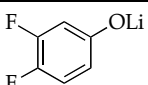
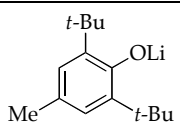
 7	DME	0.64 M	2.9 M	122
 9	DME	0.24 M	6.3 M	124
 11	DME	0.22 M	9.6 M	125
 18	DME	0.23 M	2.9 M	126

Table A1.3. (continued)

 21	DME	0.24 M	9.6 M	127
 24	DME	0.24 M	9.6 M	128
 27	DME	0.24 M	9.6 M	129
 28	DME	0.24 M	9.6 M	130
 30	DME	0.21 M	9.6 M	131
 32	DME	0.0 M (neat toluene)	0.87 M	132

IV. Phenolate concentration scans.

Solvent	Substrate	Lower limit	Upper limit	Page No.
DME	 15	0.018 N	0.109 N	134
DME	 32	0.011 N	0.229 N	136

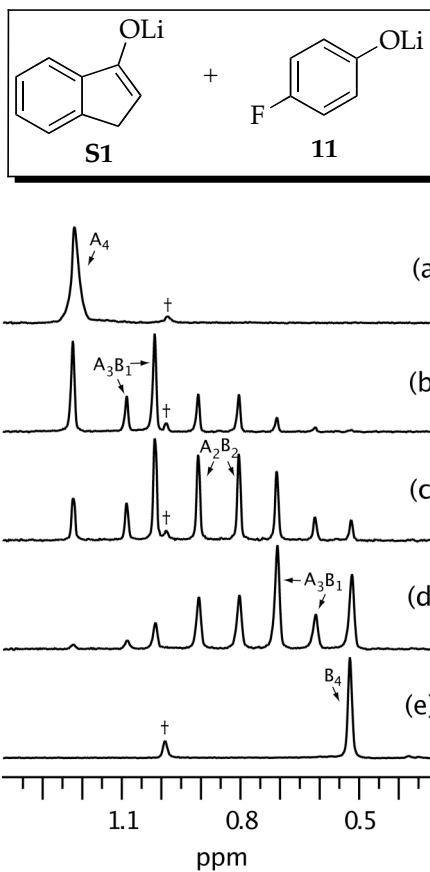


Figure A1.1. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\text{S1}$ (**A**) and $[\text{}^6\text{Li}]\text{11}$ (**B**) at 1.2 M THF/toluene at $-78\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.26, 0.45, 0.67, 1.00 respectively. † denotes excess LiHMDS dimer.

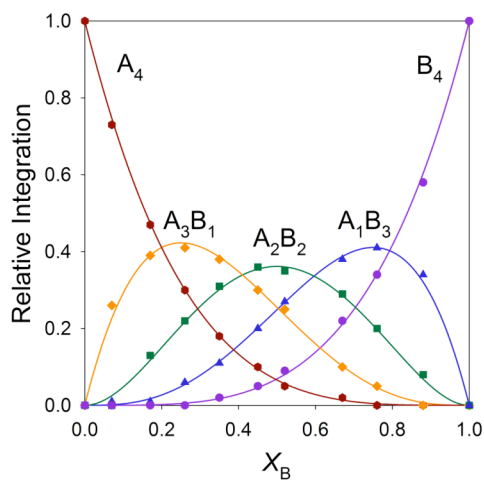


Figure A1.2. Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of $[\text{}^6\text{Li}]\text{S1}$ (**A**) and $[\text{}^6\text{Li}]\text{11}$ (**B**) in 1.2 M THF/toluene at $-78\text{ }^\circ\text{C}$.

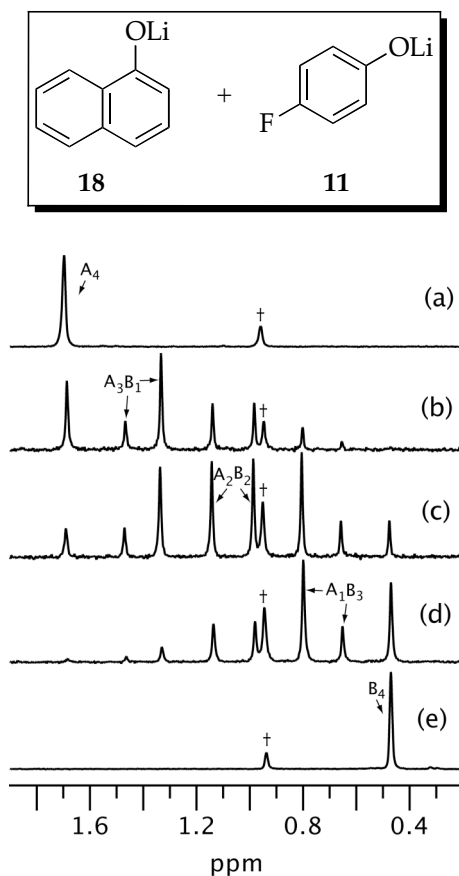


Figure A1.3. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{18}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{11}$ (**B**) at 1.2 M THF/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.30, 0.50, 0.71, 1.00 respectively. † denotes excess LiHMDS dimer.

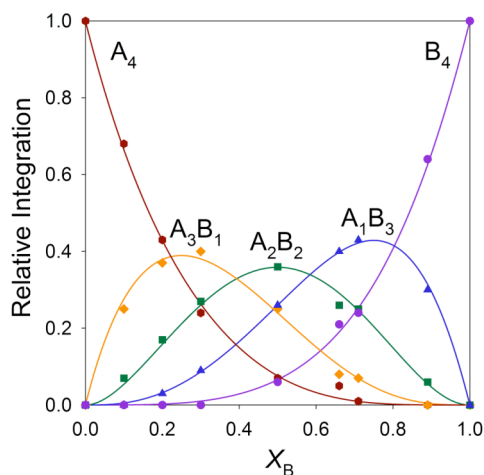


Figure A1.4. Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{18}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{11}$ (**B**) in 1.2 M THF/toluene at $-90\text{ }^\circ\text{C}$.

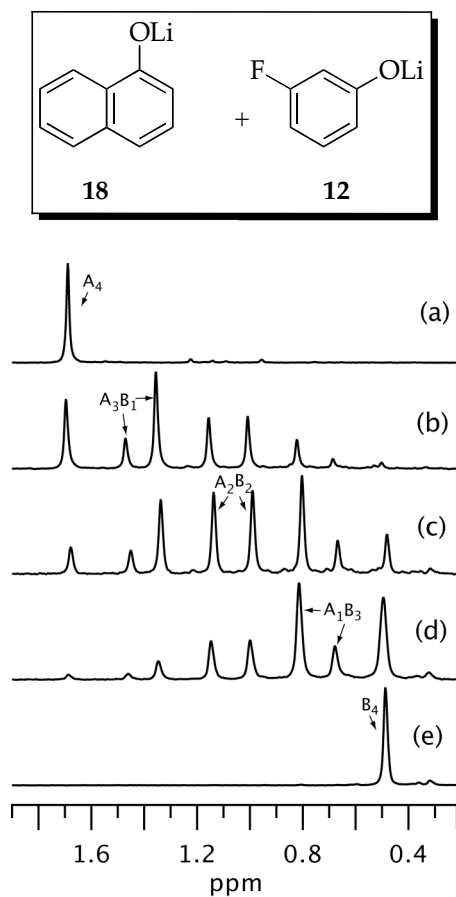


Figure A1.5. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{18}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{12}$ (**B**) at 1.2 M THF/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.35, 0.53, 0.72, 1.00 respectively.

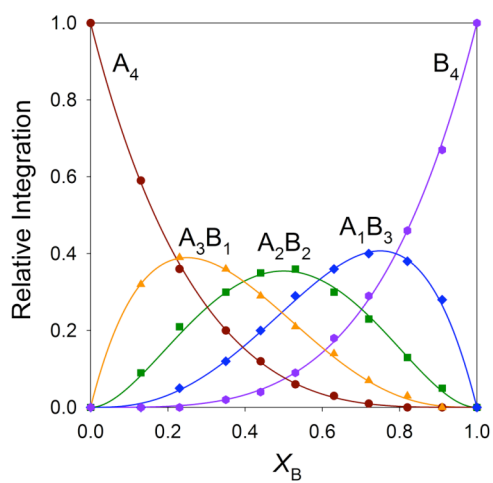


Figure A1.6. Job plot showing the relative integrations versus mole fractions of **12** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{18}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{12}$ (**B**) in 1.2 M THF/toluene at $-90\text{ }^\circ\text{C}$.

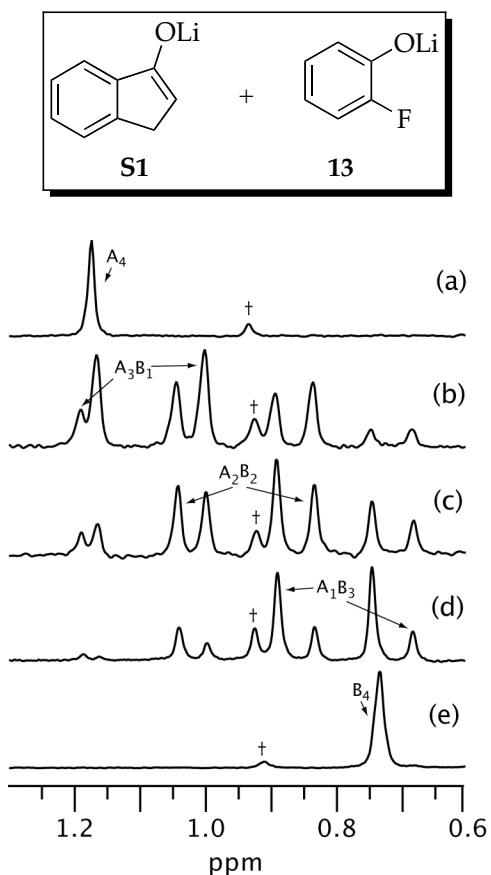


Figure A1.7. ^6Li NMR spectra of 0.10 M solutions of $[^6\text{Li}]\text{S1}$ (**A**) and $[^6\text{Li}]\text{13}$ (**B**) at 1.2 M THF/toluene at $-78\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.34, 0.55, 0.73, 1.00 respectively. † denotes excess LiHMDS dimer.

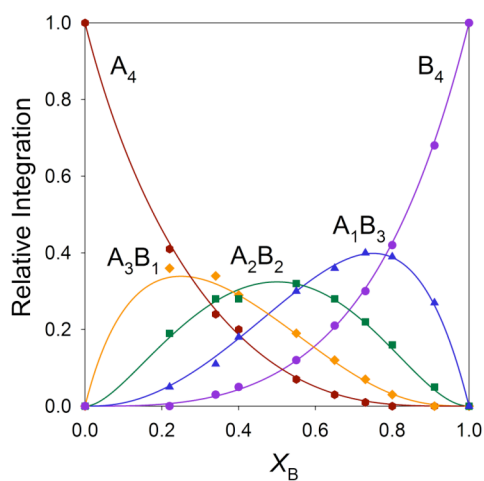


Figure A1.8. Job plot showing the relative integrations versus mole fractions of **13** for 0.10 M mixtures of $[^6\text{Li}]\text{S1}$ (**A**) and $[^6\text{Li}]\text{13}$ (**B**) in 1.2 M THF/toluene at $-78\text{ }^\circ\text{C}$.

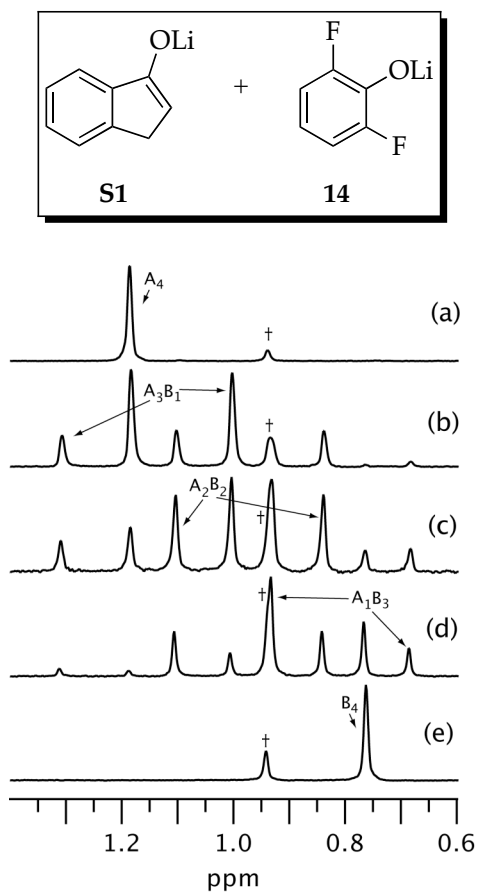


Figure A1.9. ^6Li NMR spectra of 0.10 M solutions of $[^6\text{Li}]\text{S1}$ (**A**) and $[^6\text{Li}]\text{14}$ (**B**) at 1.2 M THF/toluene at $-78\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.28, 0.46, 0.65, 1.00 respectively. † denotes excess LiHMDS dimer.

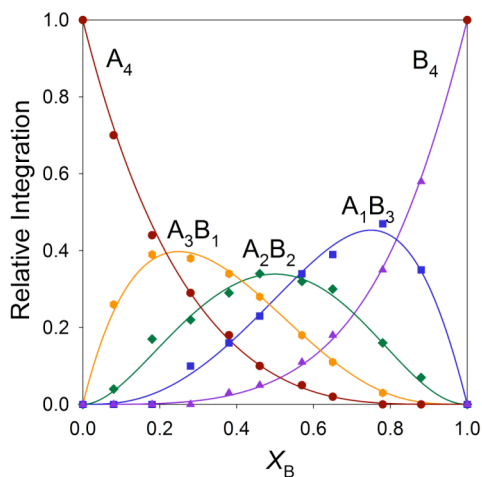


Figure A1.10. Job plot showing the relative integrations versus mole fractions of **14** for 0.10 M mixtures of enolates $[^6\text{Li}]\text{S1}$ (**A**) and $[^6\text{Li}]\text{14}$ (**B**) in 1.2 M THF/toluene at $-78\text{ }^\circ\text{C}$.

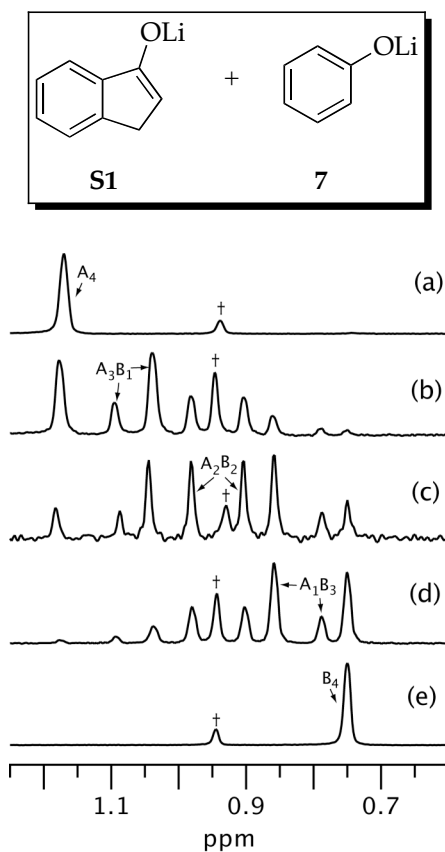


Figure A1.11. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\text{S1}$ (**A**) and $[\text{}^6\text{Li}]\text{7}$ (**B**) at 1.2 M THF/toluene at $-78\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.30, 0.50, 0.69, 1.00 respectively. † denotes excess LiHMDS dimer.

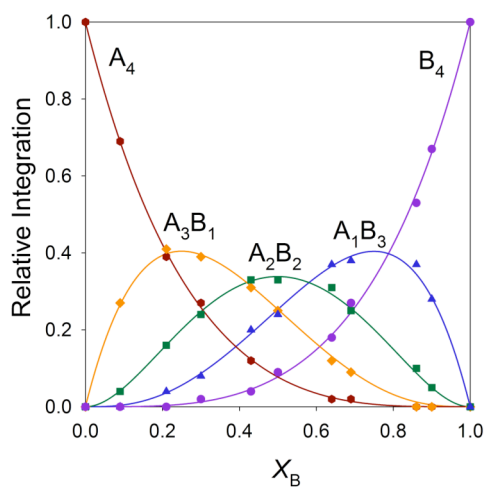


Figure A1.12. Job plot showing the relative integrations versus mole fractions of **7** for 0.10 M mixtures of $[\text{}^6\text{Li}]\text{S1}$ (**A**) and $[\text{}^6\text{Li}]\text{7}$ (**B**) in 1.2 M THF/toluene at $-78\text{ }^\circ\text{C}$.

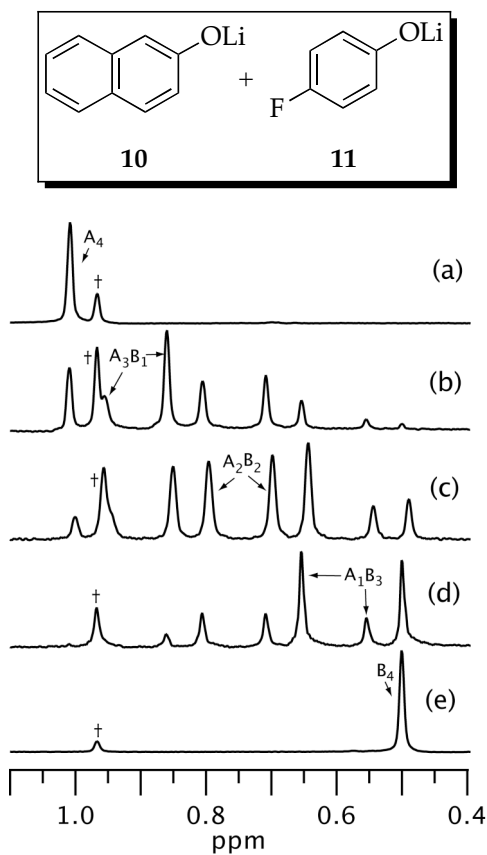


Figure A1.13. ^6Li NMR spectra of 0.10 M solutions of $[^6\text{Li}]\mathbf{10}$ (**A**) and $[^6\text{Li}]\mathbf{11}$ (**B**) at $-78\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.35, 0.53, 0.73, 1.00 respectively. † denotes excess LiHMDS dimer.

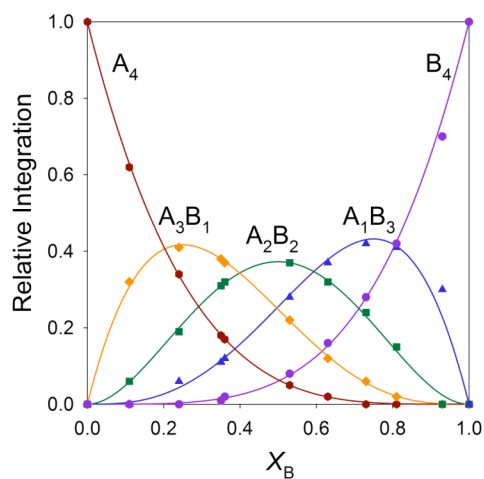


Figure A1.14. Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of phenolates $[^6\text{Li}]\mathbf{10}$ (**A**) and $[^6\text{Li}]\mathbf{11}$ (**B**) in 1.2 M THF/toluene at $-78\text{ }^\circ\text{C}$.

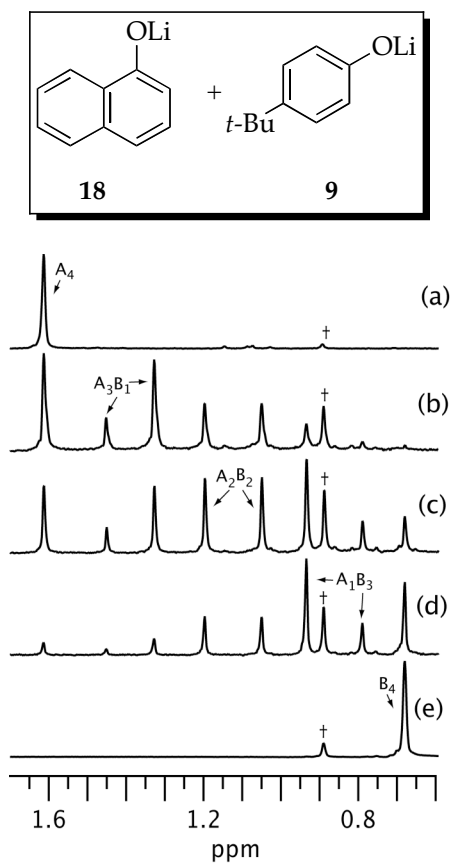


Figure A1.15. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{18}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{9}$ (**B**) at 1.2 M THF/toluene at $-78\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.31, 0.49, 0.69, 1.00 respectively. † denotes excess LiHMDS dimer.

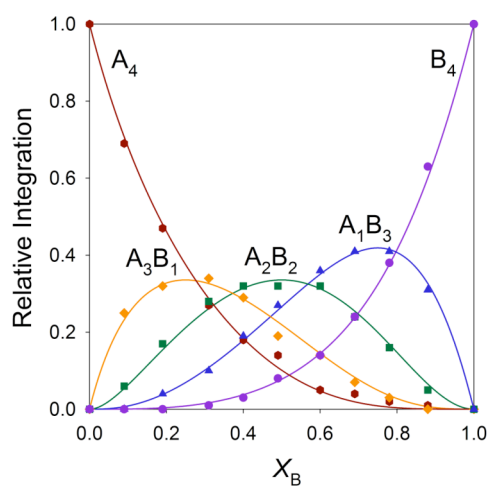


Figure A1.16. Job plot showing the relative integrations versus mole fractions of **9** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{18}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{9}$ (**B**) in 1.2 M THF/toluene at $-78\text{ }^\circ\text{C}$.

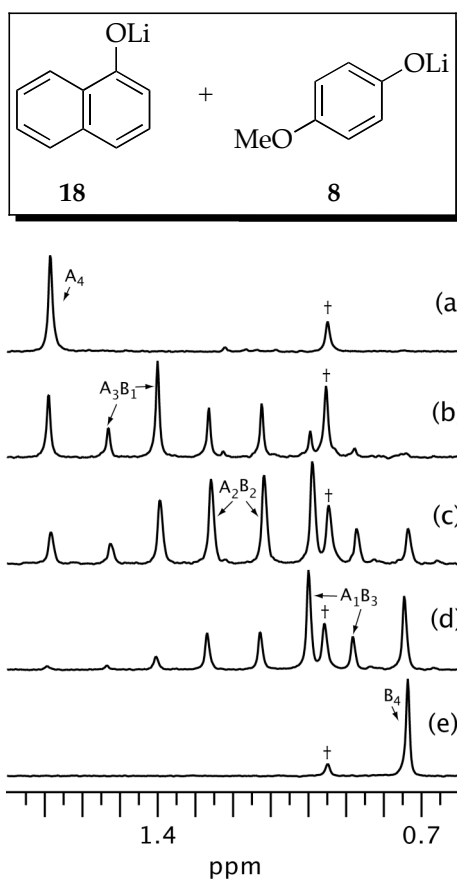


Figure A1.17. ^6Li NMR spectra of 0.10 M solutions of $[^6\text{Li}]\mathbf{18}$ (**A**) and $[^6\text{Li}]\mathbf{8}$ (**B**) at 1.2 M THF/toluene at -90°C . The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.35, 0.53, 0.70, 1.0 respectively. † denotes excess LiHMDS dimer.

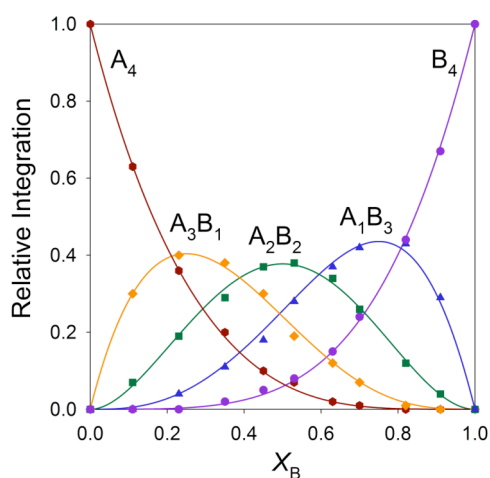


Figure A1.18. Job plot showing the relative integrations versus mole fractions of **8** for 0.10 M mixtures of phenolates $[^6\text{Li}]\mathbf{18}$ (**A**) and $[^6\text{Li}]\mathbf{8}$ (**B**) in 1.2 M THF/toluene at -90°C .

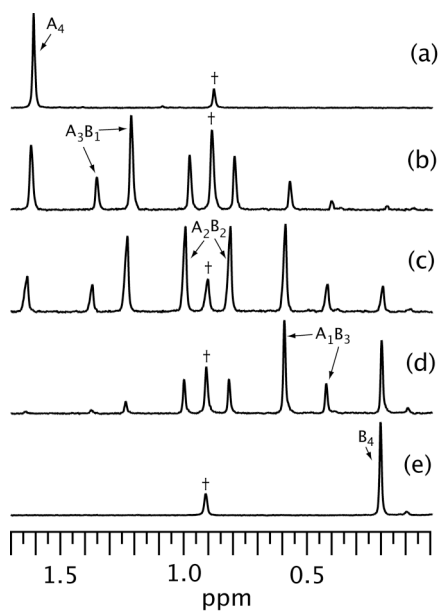
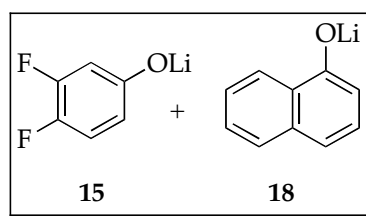


Figure A1.19. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{18}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{15}$ (**B**) at 1.2 M THF/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.33, 0.49, 0.72, 1.00 respectively. † denotes excess LiHMDS dimer.

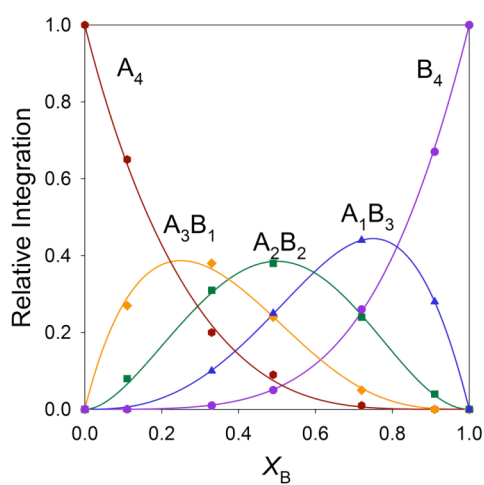


Figure A1.20. Job plot showing the relative integrations versus mole fractions of **18** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{18}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{15}$ (**B**) in 1.2 M THF/toluene at $-90\text{ }^\circ\text{C}$.

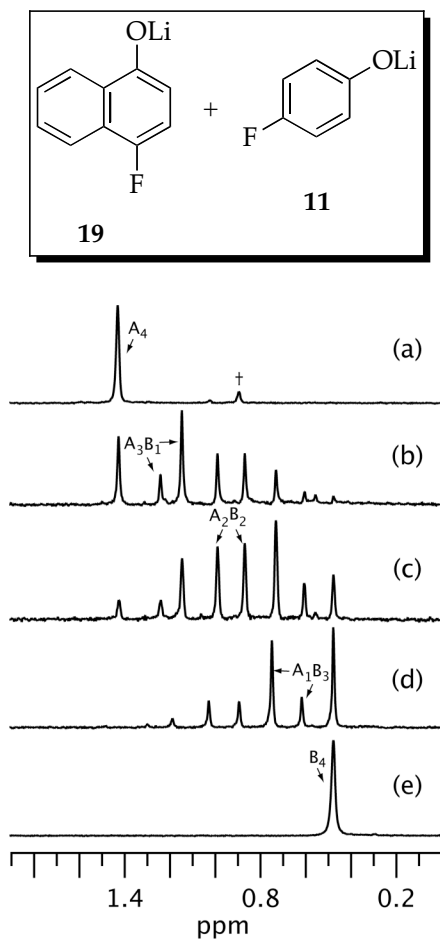


Figure A1.21. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\textbf{19}$ (**A**) and $[\text{}^6\text{Li}]\textbf{11}$ (**B**) at 1.2 M THF/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.37, 0.55, 0.77, 1.00 respectively. \dagger denotes excess LiHMDS dimer.

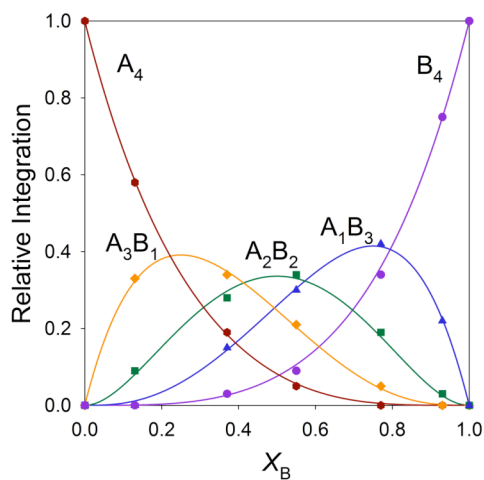
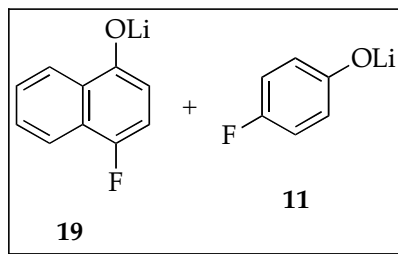


Figure A1.22. Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of phenolates [^6Li]**19**(A) and [^6Li]**15**(B) in 1.2 M THF/toluene at $-90\text{ }^\circ\text{C}$. The non-statistical behavior of the Job plot may stem from low solubility of **19** in 1.2 M THF/toluene at $-90\text{ }^\circ\text{C}$.

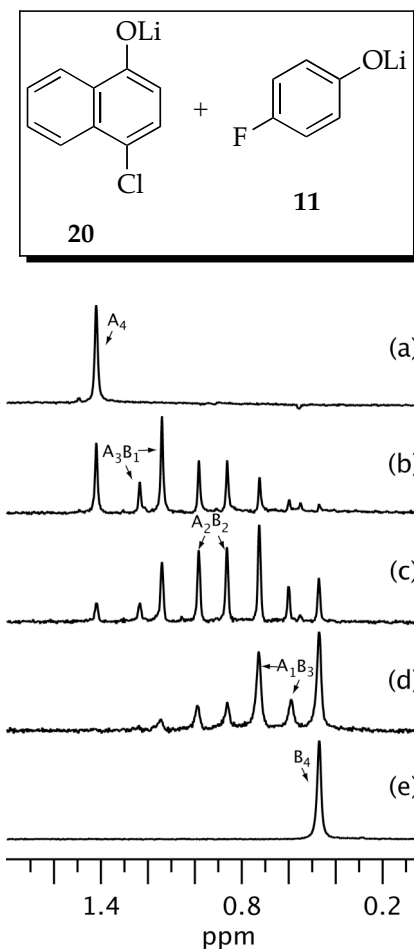


Figure A1.23. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{20}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{11}$ (**B**) at 1.2 M THF/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.37, 0.55, 0.76, 1.00 respectively.

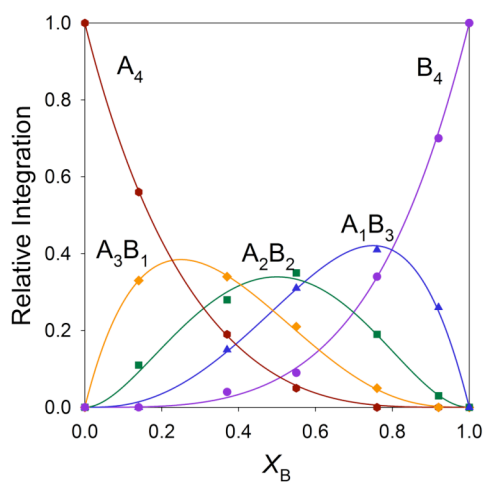


Figure A1.24. Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{20}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{11}$ (**B**) in 1.2 M THF/toluene at $-90\text{ }^\circ\text{C}$.

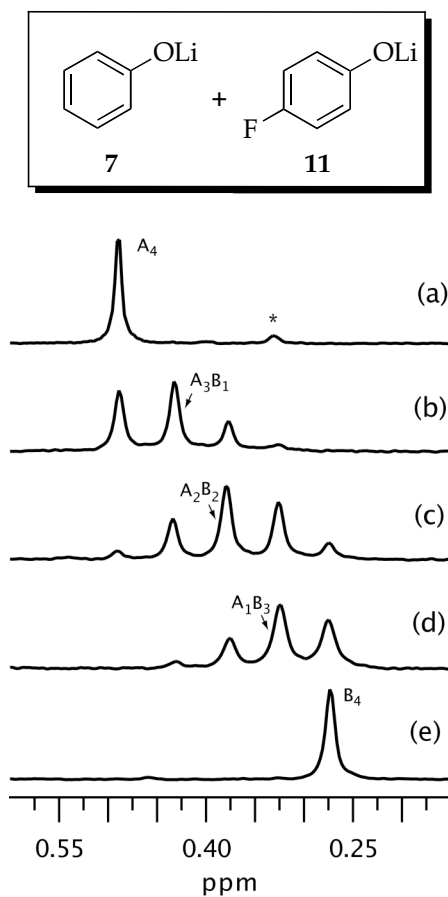


Figure A1.25. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{7}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{11}$ (**B**) at 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.24, 0.54, 0.75, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate.

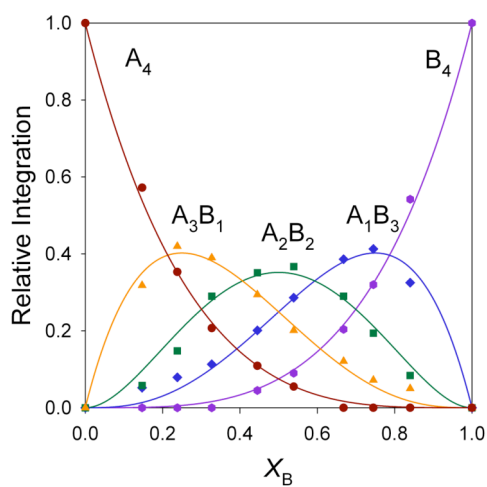


Figure A1.26. Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{7}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{11}$ (**B**) in 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$.

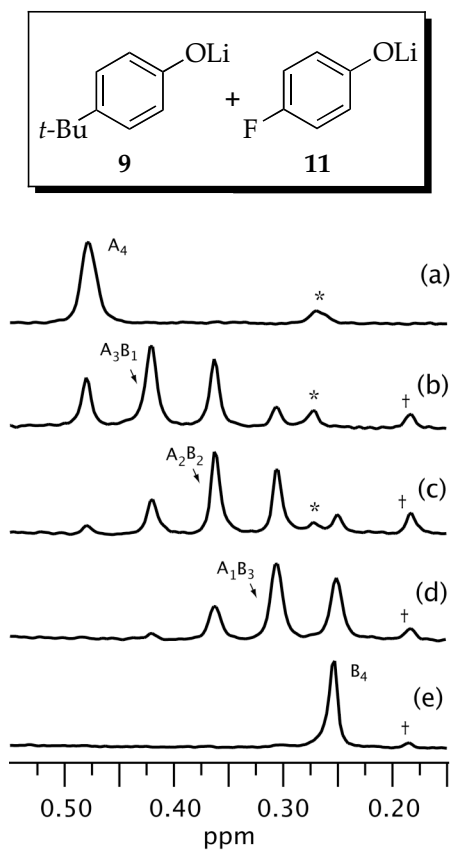


Figure A1.27. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{9}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{11}$ (**B**) at 2.9 M DME/toluene at $-70\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.31, 0.53, 0.75, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate; † denotes **B**·LiHMDS mixed aggregate.

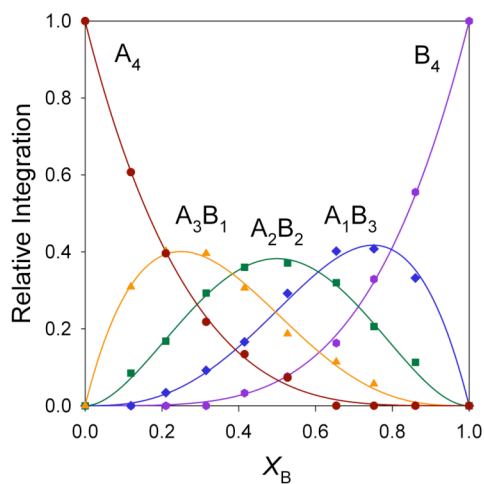


Figure A1.28. Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{9}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{11}$ (**B**) in 2.9 M DME/toluene at $-70\text{ }^\circ\text{C}$.

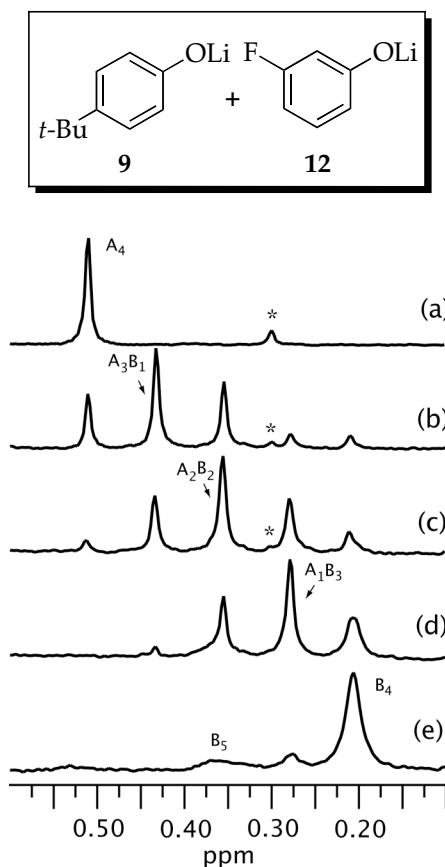


Figure A1.29. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{9}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{12}$ (**B**) at 2.9 M DME/toluene at $-70\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.34, 0.52, 0.72, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate.

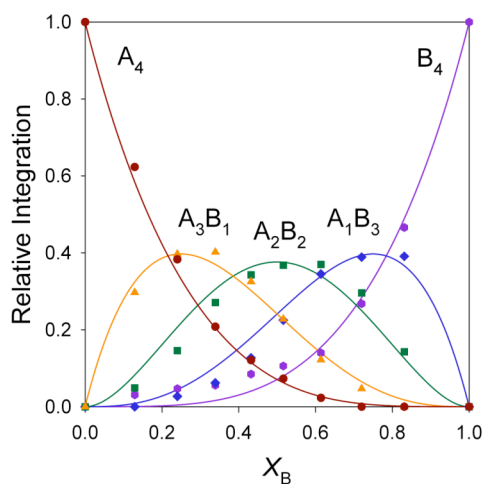


Figure A1.30. Job plot showing the relative integrations versus mole fractions of **12** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{9}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{12}$ (**B**) in 2.9 M DME/toluene at $-70\text{ }^\circ\text{C}$.

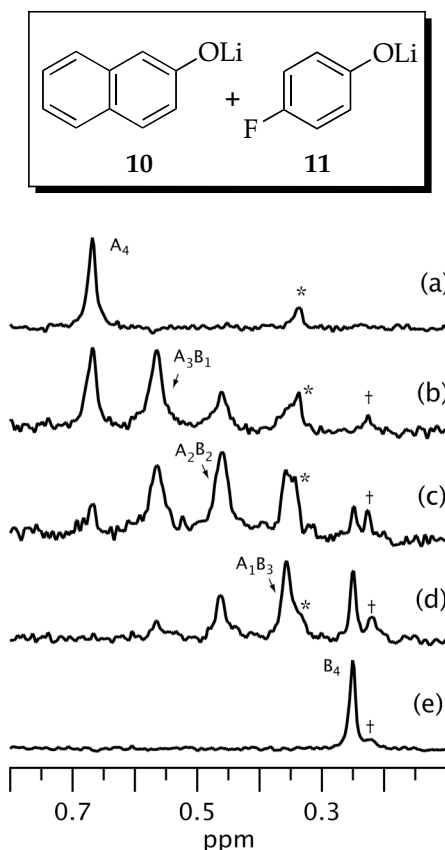


Figure A1.31. ^6Li NMR spectra of 0.10 M solutions of $[^6\text{Li}]\mathbf{10}$ (**A**) and $[^6\text{Li}]\mathbf{11}$ (**B**) at 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.24, 0.47, 0.66, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate; † denotes **B**·LiHMDS mixed aggregate.

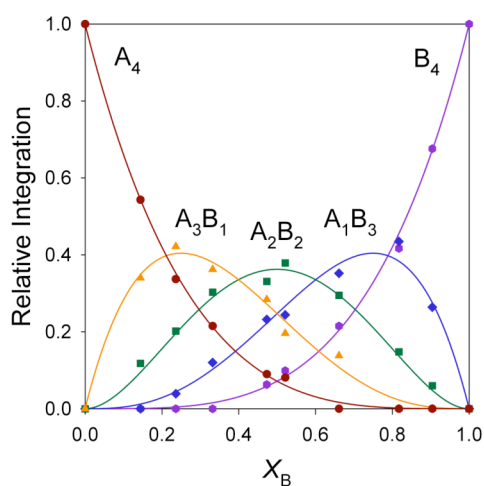


Figure A1.32. Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of phenolates $[^6\text{Li}]\mathbf{10}$ (**A**) and $[^6\text{Li}]\mathbf{11}$ (**B**) in 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$.

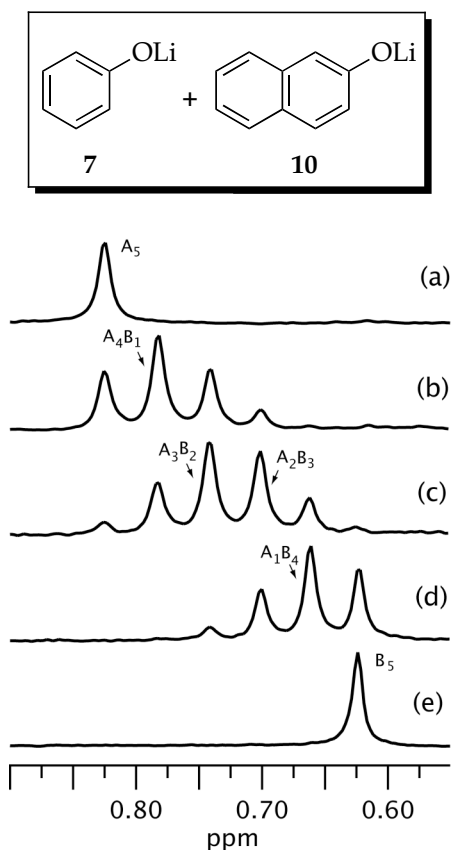


Figure A1.33 ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\textbf{7}$ (**A**) and $[\text{}^6\text{Li}]\textbf{10}$ (**B**) at 0.22 M DME/toluene at $-30\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.24, 0.45, 0.78, 1.00 respectively.

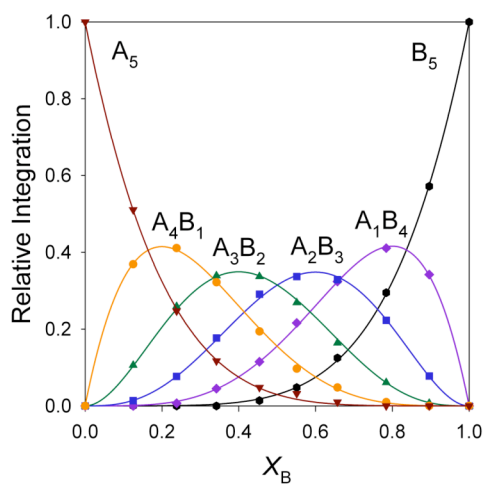


Figure A1.34. Job plot showing the relative integrations versus mole fractions of **10** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\textbf{7}$ (**A**) and $[\text{}^6\text{Li}]\textbf{10}$ (**B**) in 0.22 M DME/toluene at $-30\text{ }^\circ\text{C}$.

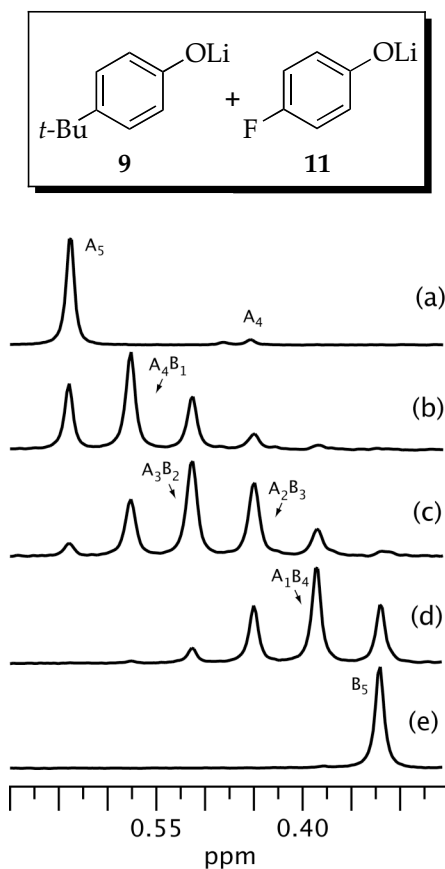


Figure A1.35. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{9}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{11}$ (**B**) at 0.22 M DME/toluene at $-30\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)–(e) are 0.00, 0.25, 0.45, 0.77, 1.00 respectively.

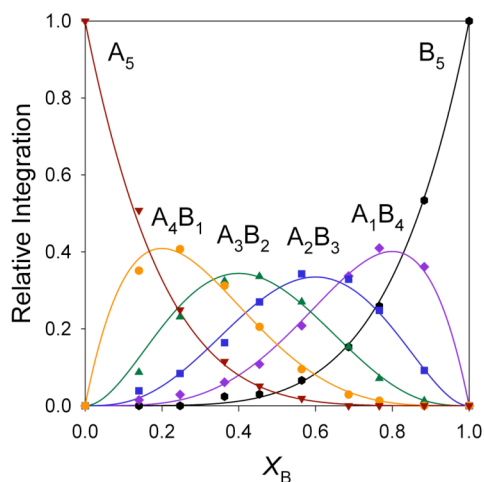


Figure A1.36. Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{9}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{11}$ (**B**) in 0.22 M DME/toluene at $-30\text{ }^\circ\text{C}$.

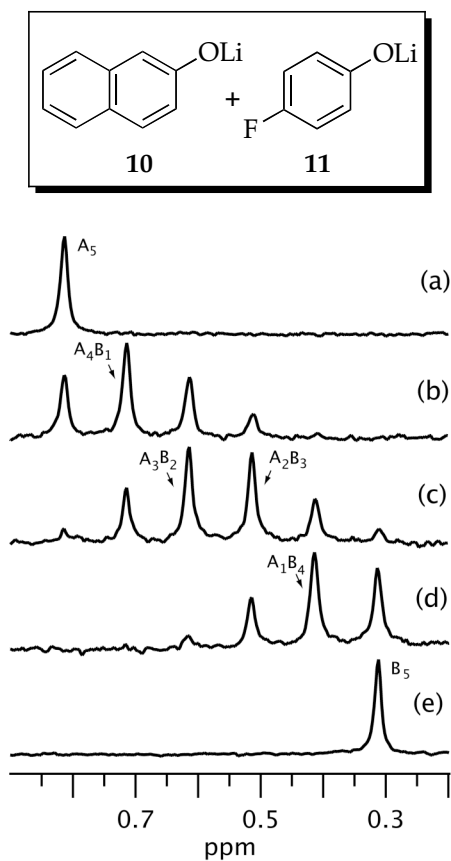


Figure A1.37. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\textbf{10}$ (**A**) and $[\text{}^6\text{Li}]\textbf{11}$ (**B**) at 0.22 M DME/toluene at $-30\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.26, 0.50, 0.79, 1.00 respectively.

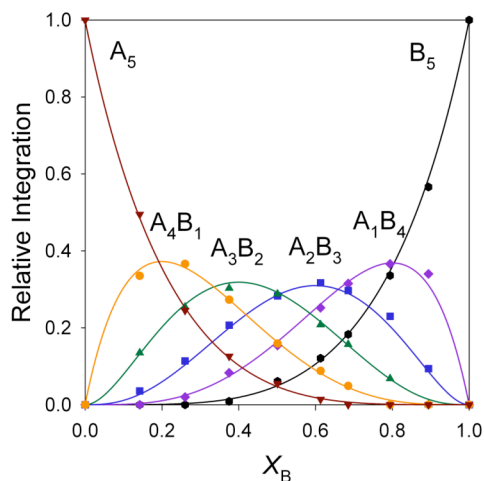


Figure A1.38. Job plot showing the relative integrations versus mole fractions of **11** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\textbf{10}$ (**A**) and $[\text{}^6\text{Li}]\textbf{11}$ (**B**) in 0.22 M DME/toluene at $-30\text{ }^\circ\text{C}$.

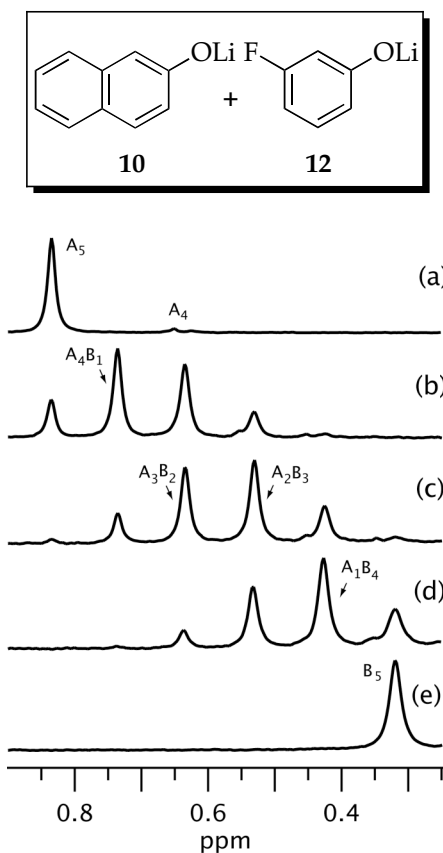


Figure A1.39. ^6Li NMR spectra of 0.10 M solutions of $[^6\text{Li}]\mathbf{10}$ (**A**) and $[^6\text{Li}]\mathbf{12}$ (**B**) at 0.22 M DME/toluene at $-30\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.30, 0.52, 0.75, 1.00 respectively.

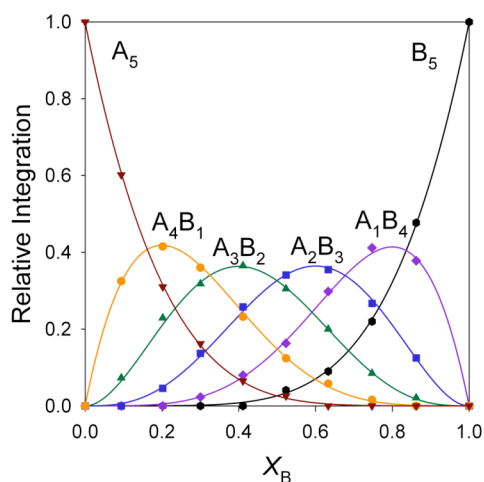


Figure A1.40. Job plot showing the relative integrations versus mole fractions of **12** for 0.10 M mixtures of phenolates $[^6\text{Li}]\mathbf{10}$ (**A**) and $[^6\text{Li}]\mathbf{12}$ (**B**) in 0.22 M DME/toluene at $-30\text{ }^\circ\text{C}$.

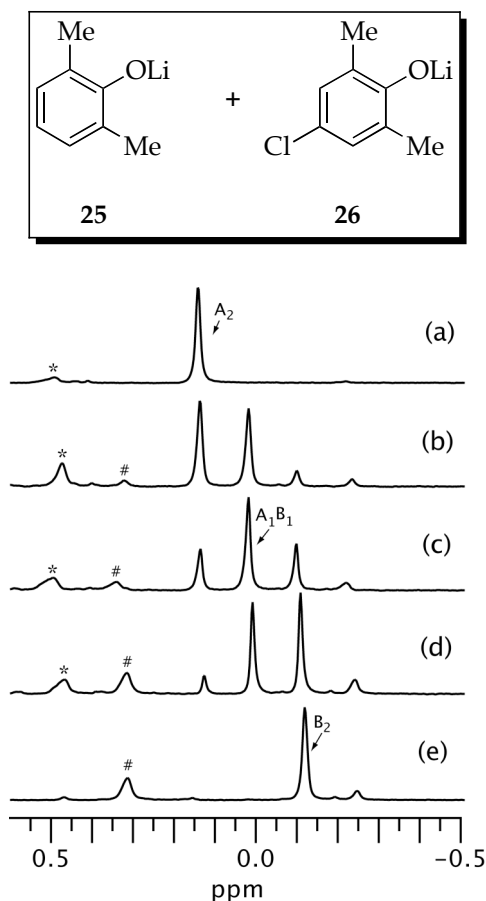


Figure A1.41. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{25}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{26}$ (**B**) at 2.0 M THF/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.30, 0.50, 0.70, 1.00 respectively. * denotes excess **A**. LiHMDS and # denotes **B**. LiHMDS.

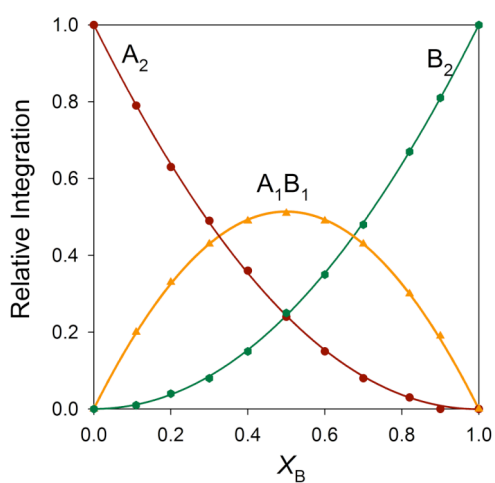


Figure A1.42. Job plot showing the relative integrations versus mole fractions of **26** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{25}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{26}$ (**B**) in 2.0 M THF/toluene at $-90\text{ }^\circ\text{C}$.

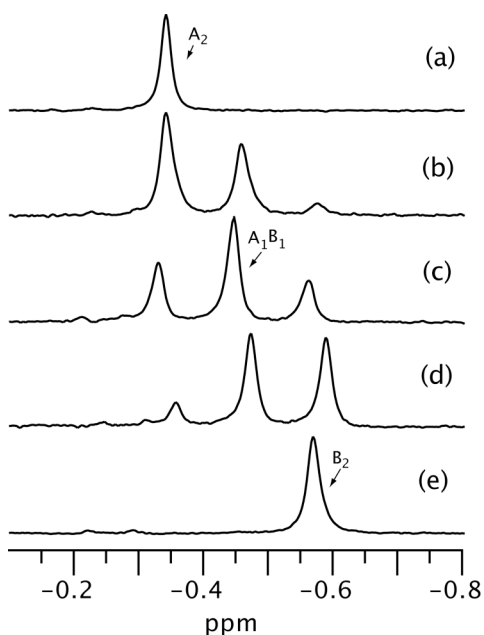


Figure 1 is a line graph showing the relative integration of three species (A_2 , B_2 , and A_1B_1) as a function of the mole fraction of B (x_B). The y-axis is labeled 'Relative Integration' and ranges from 0.0 to 1.0. The x-axis is labeled ' x_B ' and ranges from 0.0 to 1.0. The A_2 curve (red line with square markers) starts at 1.0 at $x_B = 0.0$ and decreases to 0.0 at $x_B = 1.0$. The B_2 curve (green line with triangle markers) starts at 0.0 at $x_B = 0.0$ and increases to 1.0 at $x_B = 1.0$. The A_1B_1 curve (orange line with circle markers) starts at 0.0 at $x_B = 0.0$, reaches a maximum of 0.5 at $x_B = 0.5$, and returns to 0.0 at $x_B = 1.0$.

x_B	A_2	B_2	A_1B_1
0.0	1.00	0.00	0.00
0.1	0.83	0.02	0.16
0.2	0.69	0.04	0.28
0.3	0.54	0.06	0.40
0.4	0.42	0.12	0.47
0.5	0.31	0.21	0.50
0.6	0.21	0.32	0.47
0.7	0.12	0.46	0.40
0.8	0.06	0.64	0.28
0.9	0.02	0.78	0.16
1.0	0.00	1.00	0.00

72

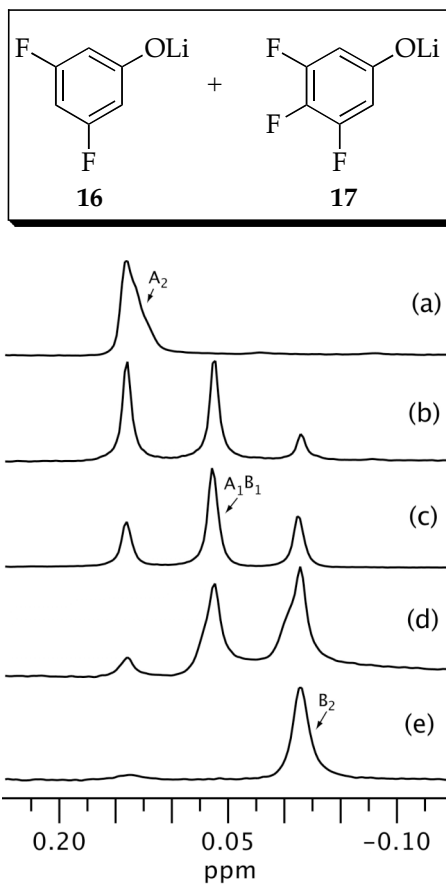


Figure A1.45. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\textbf{16}$ (**A**) and $[\text{}^6\text{Li}]\textbf{17}$ (**B**) at 3.0 M THF/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.35, 0.52, 0.70, 1.00 respectively.

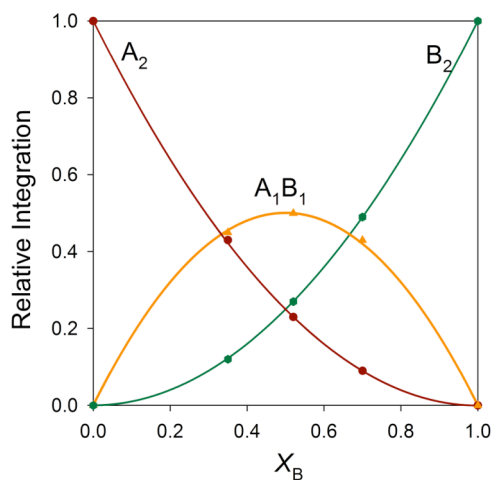


Figure A1.46. Job plot showing the relative integrations versus mole fractions of **17** for 0.10 M mixtures of penolates $[\text{}^6\text{Li}]\textbf{16}$ (**A**) and $[\text{}^6\text{Li}]\textbf{17}$ (**B**) in 3.0 M THF/toluene at $-90\text{ }^\circ\text{C}$.

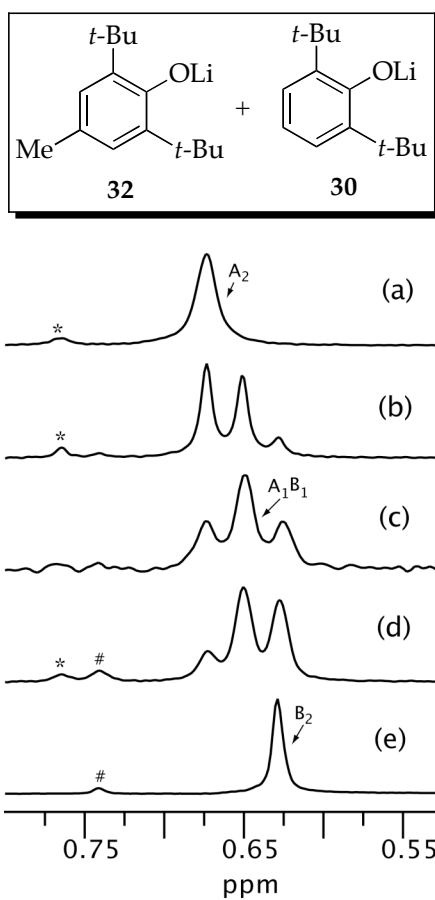


Figure A1.47. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{32}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{30}$ (**B**) at 1.2 M THF/toluene at $-78\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.33, 0.50, 0.73, 1.00 respectively. * denotes excess **A**·LiHMDS and # denotes **B**·LiHMDS mixed aggregates.

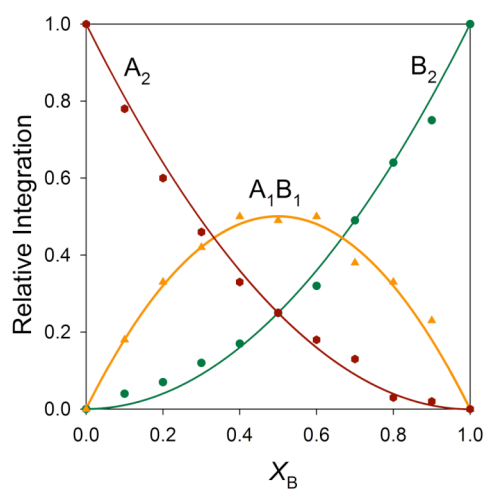
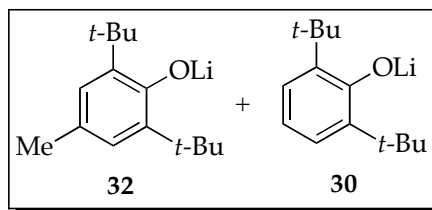


Figure A1.48. Job plot showing the relative integrations versus mole fractions of **30** for 0.10 M mixtures of phenolates $[^6\text{Li}]\mathbf{32}$ (**A**) and $[^6\text{Li}]\mathbf{32}$ (**B**) in 1.2 M THF/toluene at -78°C .

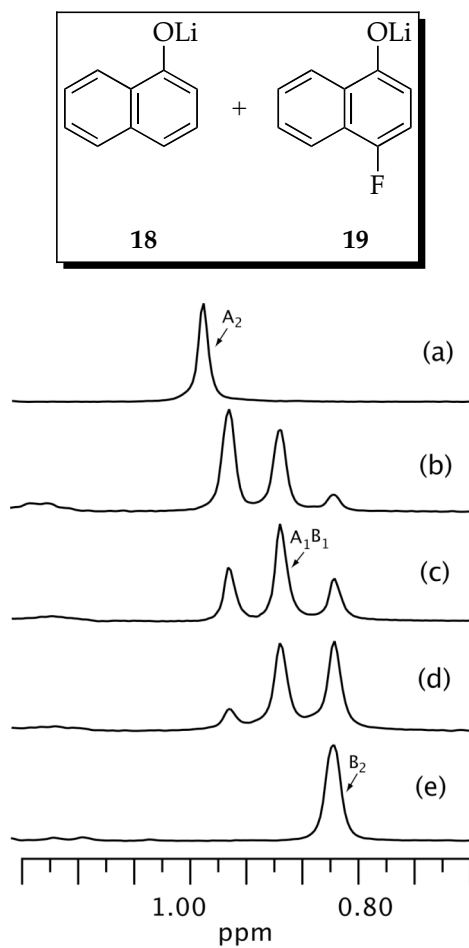


Figure A1.49. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{18}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{19}$ (**B**) at 12.2 M THF at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.27, 0.48, 0.65, 1.00 respectively.

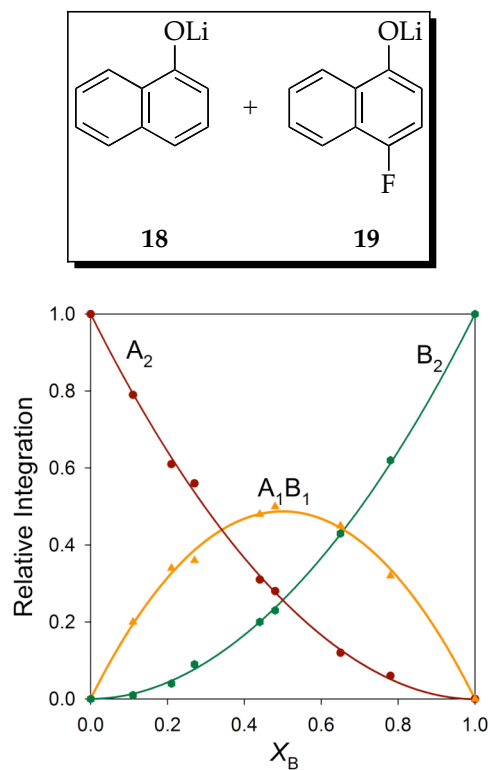


Figure A1.50. Job plot showing the relative integrations versus mole fractions of **18** for 0.10 M mixtures of phenolates [^6Li]**18** (**A**) and [^6Li]**19** (**B**) in 1.2 M THF/toluene at $-90\text{ }^\circ\text{C}$.

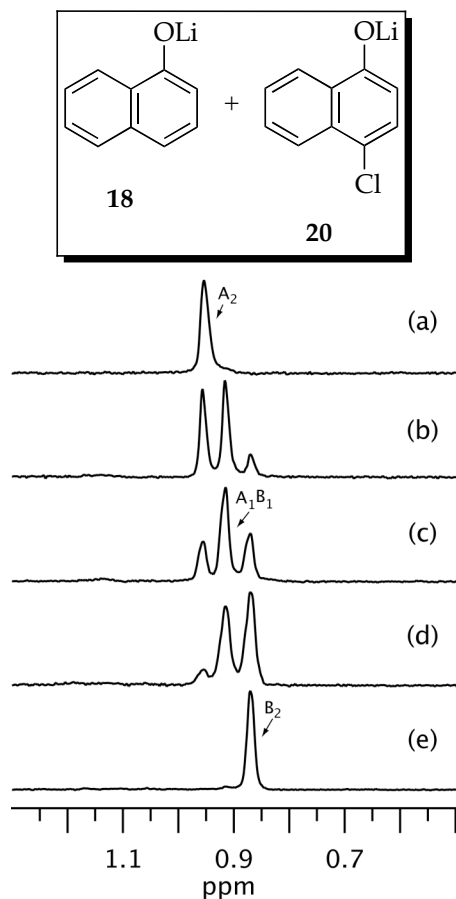


Figure A1.51. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{18}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{20}$ (**B**) in neat THF (12.2 M) at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.36, 0.53, 0.70, 1.00 respectively.

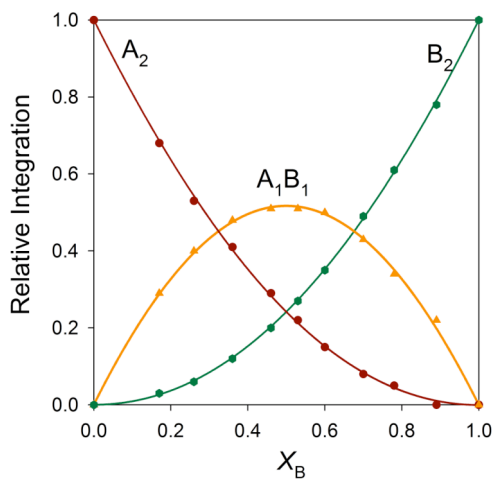


Figure A1.52. Job plot showing the relative integrations versus mole fractions of **20** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{18}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{20}$ (**B**) in neat THF (12.2 M) at $-90\text{ }^\circ\text{C}$.

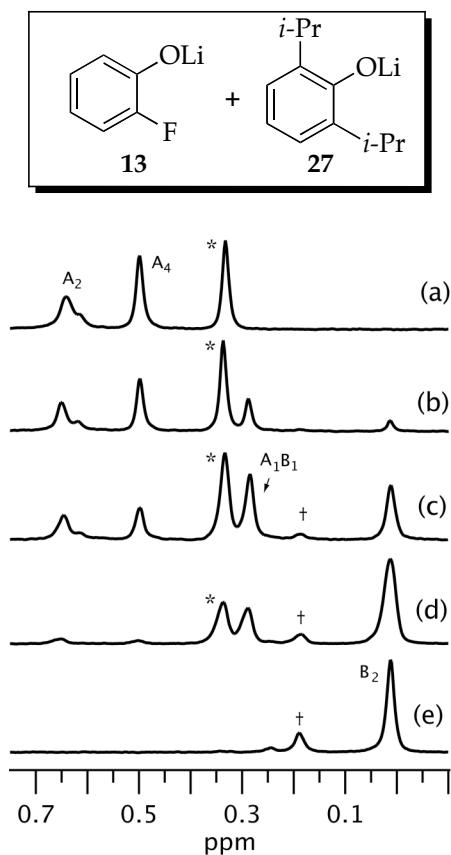


Figure A1.53. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{13}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{27}$ (**B**) at 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** within the dimer ensemble in the tubes (a)-(e) are 0.00, 0.31, 0.57, 0.82, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate; † denotes **B**·LiHMDS mixed aggregate.

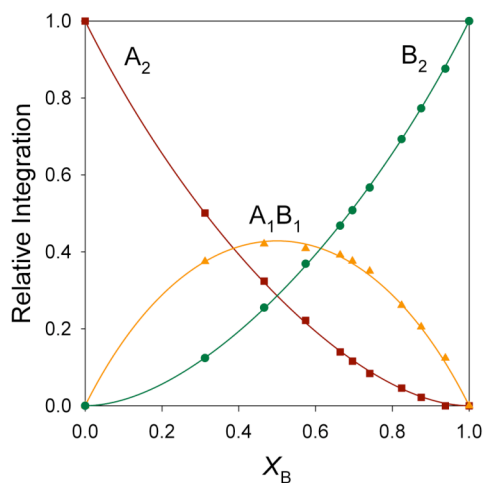
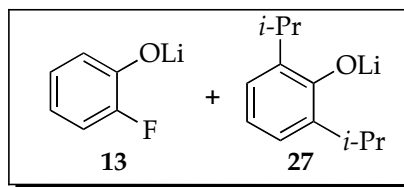


Figure A1.54. Job plot showing the relative integrations versus mole fractions of **27** (within the dimer ensemble) for 0.10 M mixtures of phenolates $[^6\text{Li}]\mathbf{13}$ (**A**) and $[^6\text{Li}]\mathbf{27}$ (**B**) in 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$. The data are skewed toward higher χ_B because the effective concentration of **13** is reduced by (a) preferential formation of its LiHMDS aggregate and (b) its tetramer homoaggregate.

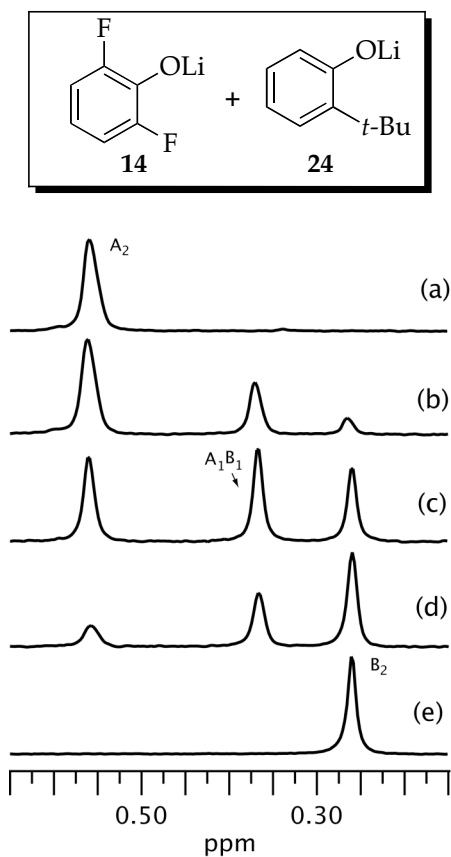


Figure A1.55. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{14}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{24}$ (**B**) at 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.23, 0.47, 0.68, 1.00 respectively.

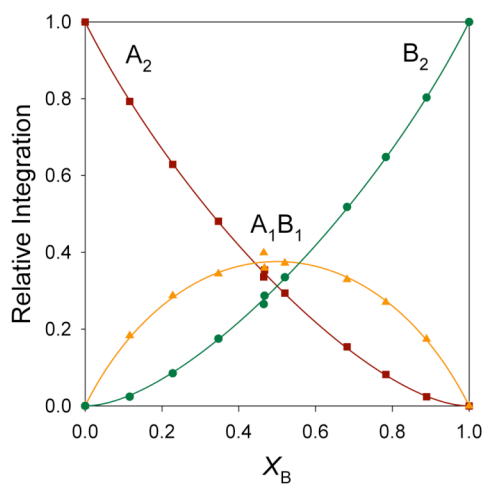


Figure A1.56. Job plot showing the relative integrations versus mole fractions of **24** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{14}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{24}$ (**B**) in 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$.

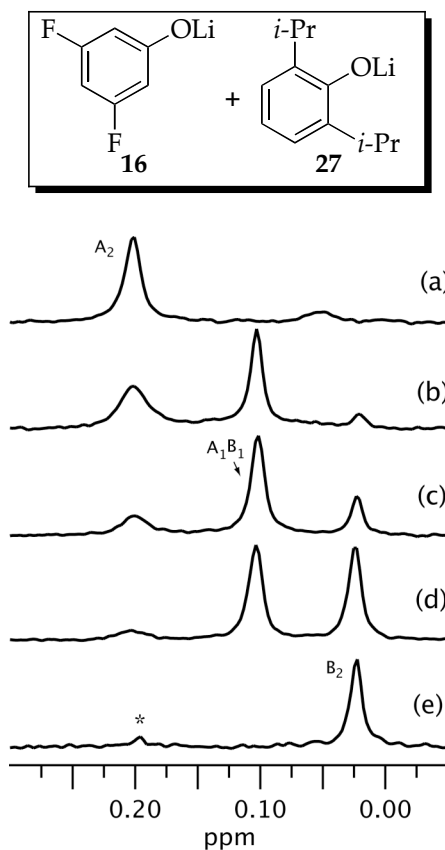


Figure A1.57. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{16}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{27}$ (**B**) at 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.34, 0.50, 0.66, 1.00 respectively. * denotes **B**·LiHMDS mixed aggregate.

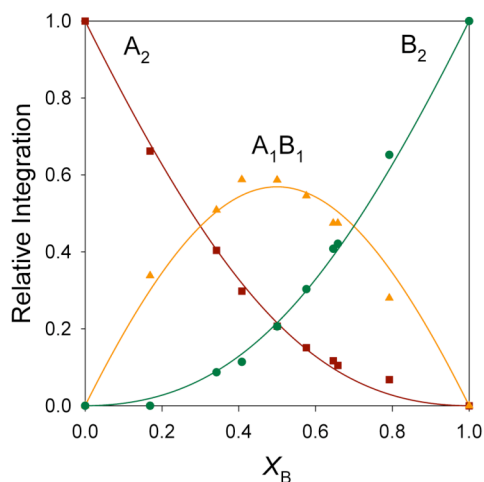


Figure A1.58. Job plot showing the relative integrations versus mole fractions of **27** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{16}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{27}$ (**B**) in 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$.

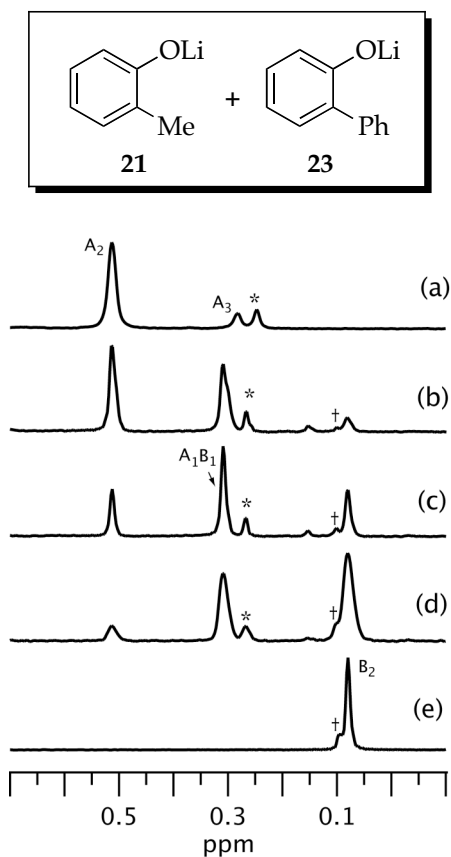


Figure A1.59. ^6Li NMR spectra of 0.10 M solutions of $[^6\text{Li}]\mathbf{21}$ (**A**) and $[^6\text{Li}]\mathbf{23}$ (**B**) at 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.30, 0.51, 0.73, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate; † denotes **B**·LiHMDS mixed aggregate.

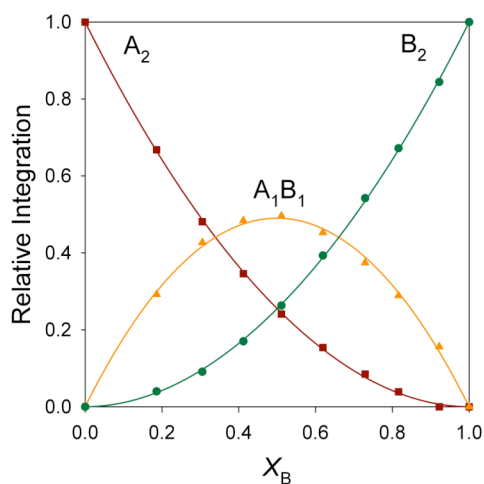


Figure A1.60. Job plot showing the relative integrations versus mole fractions of **23** for 0.10 M mixtures of phenolates $[^6\text{Li}]\mathbf{21}$ (**A**) and $[^6\text{Li}]\mathbf{23}$ (**B**) in 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$.

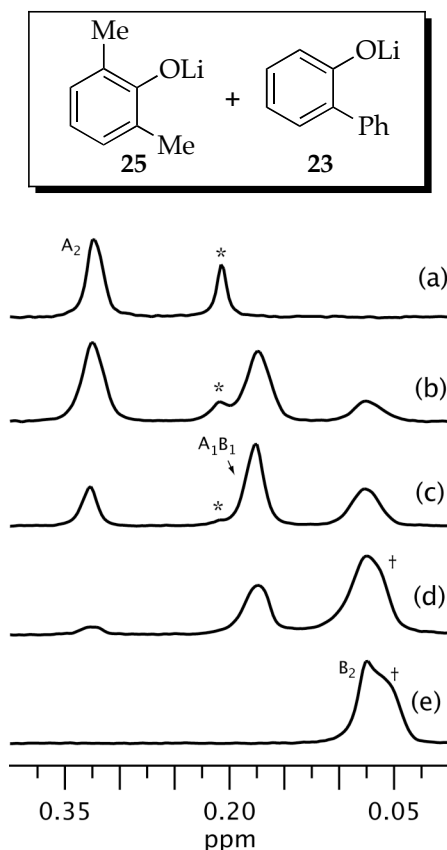


Figure A1.61. ^6Li NMR spectra of 0.10 M solutions of $[^6\text{Li}]\mathbf{25}$ (**A**) and $[^6\text{Li}]\mathbf{23}$ (**B**) at 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.30, 0.48, 0.77, 1.00 respectively. * denotes $\mathbf{A}\cdot\text{LiHMDS}$ mixed aggregate; † denotes $\mathbf{B}\cdot\text{LiHMDS}$ mixed aggregate.

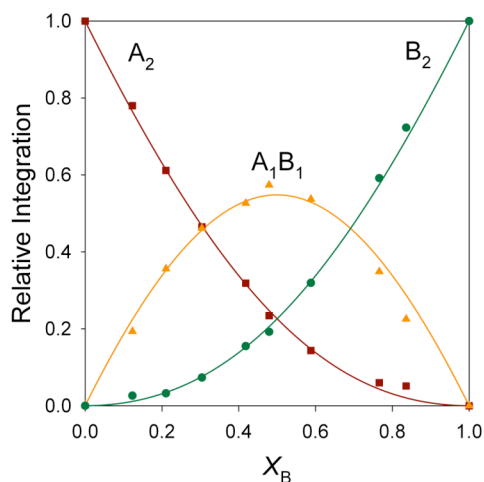


Figure A1.62. Job plot showing the relative integrations versus mole fractions of **23** for 0.10 M mixtures of phenolates $[^6\text{Li}]\mathbf{25}$ (**A**) and $[^6\text{Li}]\mathbf{23}$ (**B**) in 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$.

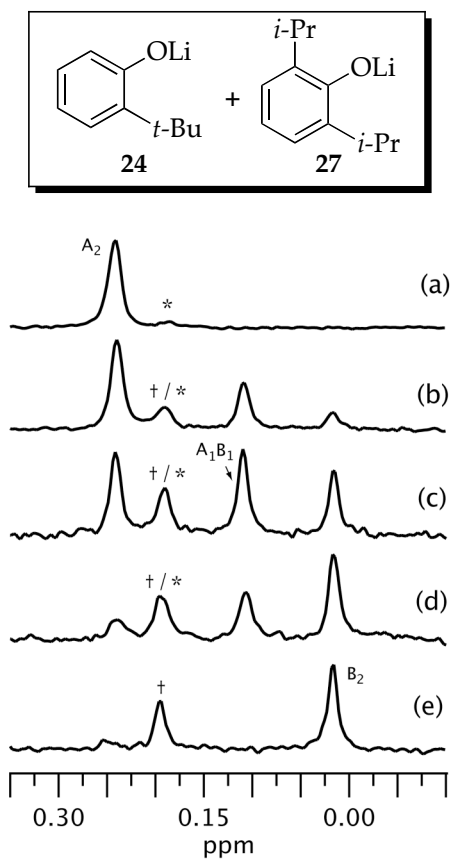


Figure A1.63. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{24}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{27}$ (**B**) at 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.26, 0.40, 0.68, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate; † denotes **B**·LiHMDS mixed aggregate.

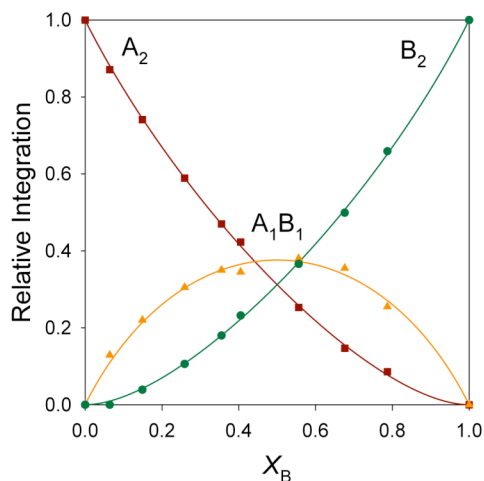


Figure A1.64. Job plot showing the relative integrations versus mole fractions of **27** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{24}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{27}$ (**B**) in 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$.

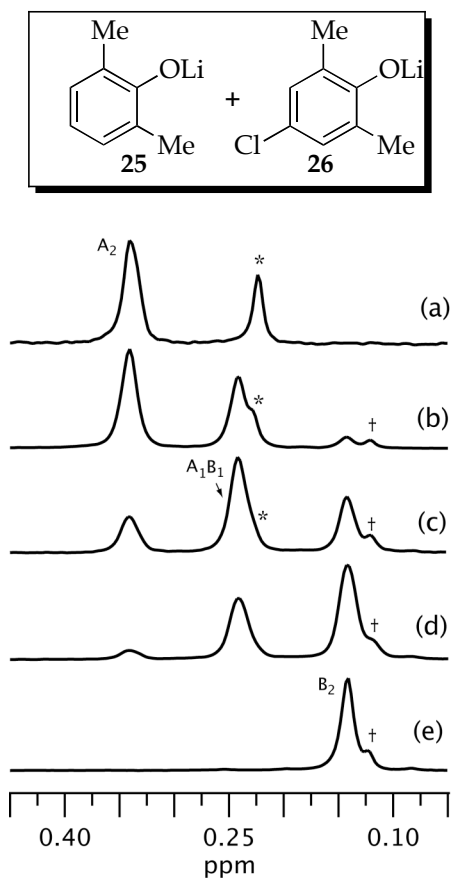


Figure A1.65. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{25}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{26}$ (**B**) at 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.24, 0.53, 0.74, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate; † denotes **B**·LiHMDS mixed aggregate.

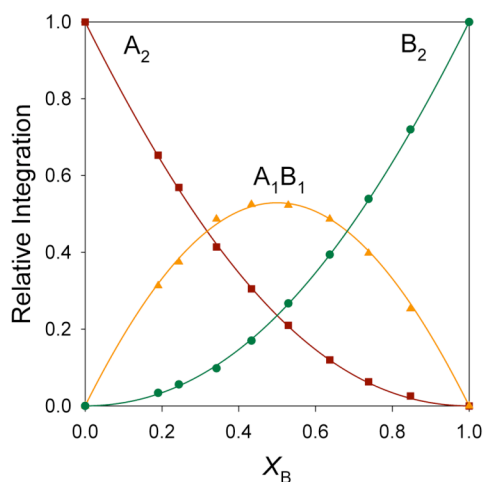


Figure A1.66. Job plot showing the relative integrations versus mole fractions of **26** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{25}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{26}$ (**B**) in 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$.

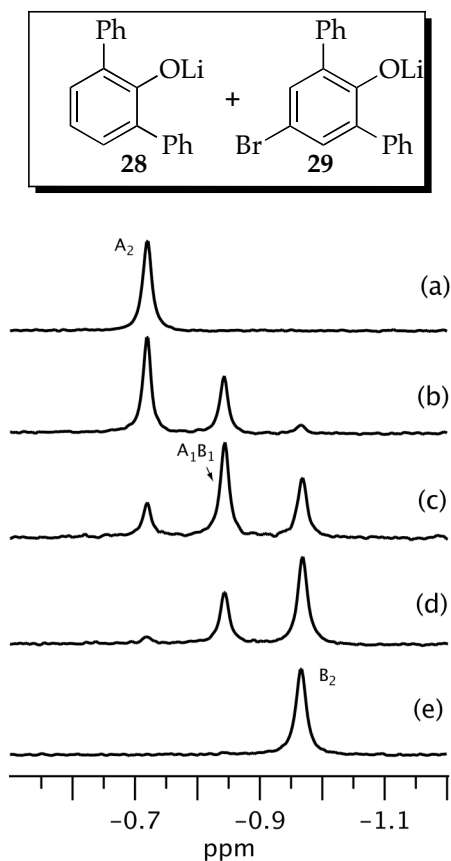


Figure A1.67. ^6Li NMR spectra of 0.05 M solutions of $[\text{}^6\text{Li}]\textbf{28}$ (**A**) and $[\text{}^6\text{Li}]\textbf{29}$ (**B**) at 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.24, 0.56, 0.76, 1.00 respectively.

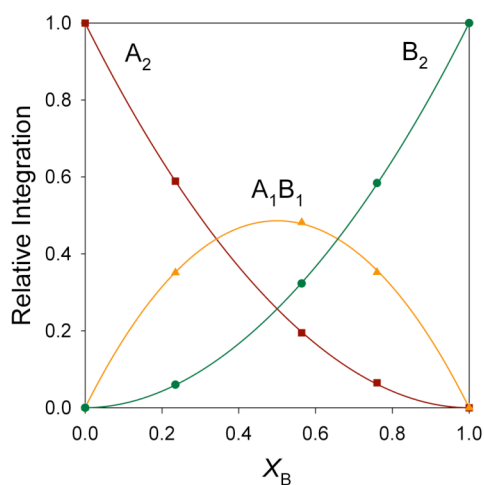


Figure A1.68. Job plot showing the relative integrations versus mole fractions of **29** for 0.05 M mixtures of phenolates $[\text{}^6\text{Li}]\textbf{28}$ (**A**) and $[\text{}^6\text{Li}]\textbf{29}$ (**B**) in 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$.

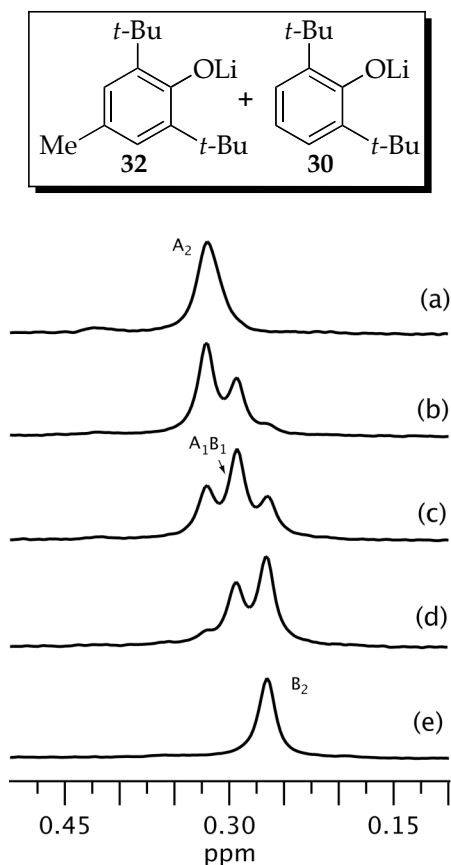


Figure A1.69. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{32}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{30}$ (**B**) at 0.22 M DME/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.24, 0.50, 0.79, 1.00 respectively.

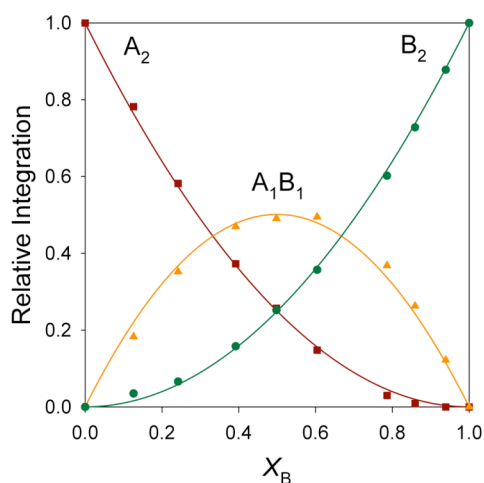


Figure A1.70. Job plot showing the relative integrations versus mole fractions of **30** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{32}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{30}$ (**B**) in 0.22 M DME/toluene at $-90\text{ }^\circ\text{C}$.

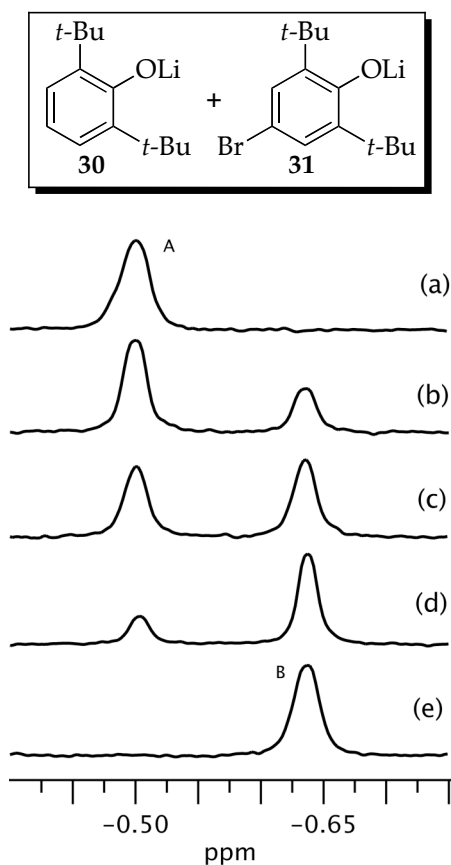


Figure A1.71. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{30}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{31}$ (**B**) at 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$. The intended mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.34, 0.56, 0.78, 1.00 respectively.

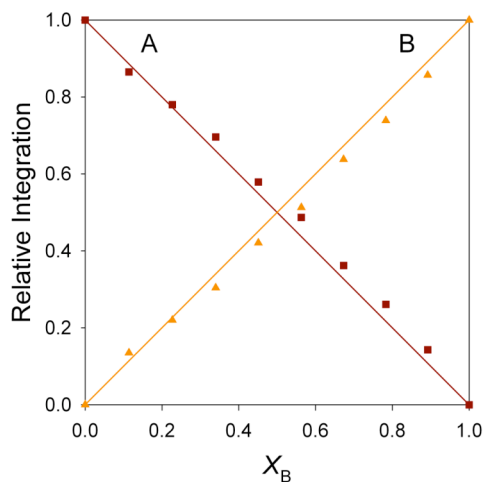


Figure A1.72. Job plot showing the relative integrations versus intended mole fractions of **31** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{30}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{31}$ (**B**) in 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$.

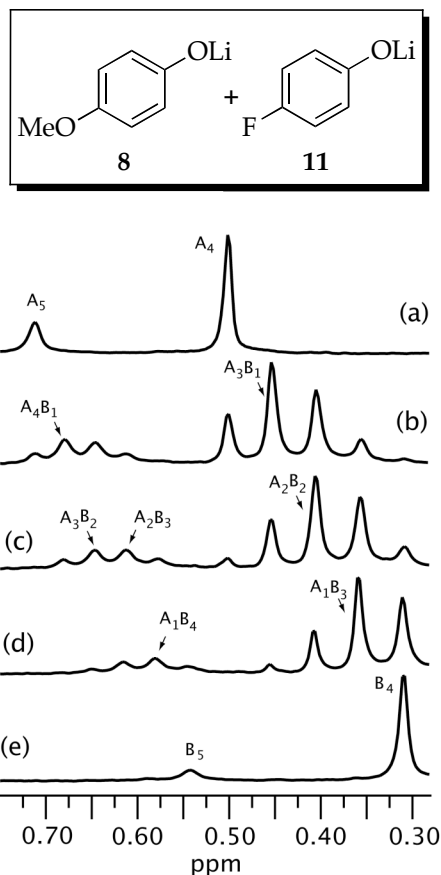


Figure A1.73. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{8}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{11}$ (**B**) at 2.9 M DME/toluene at $-50\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.36, 0.57, 0.77, 1.00 respectively.

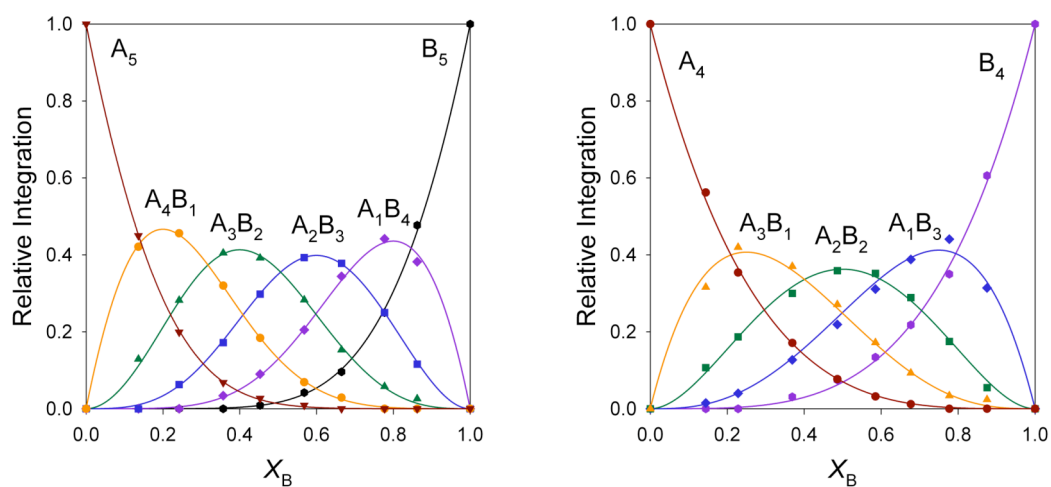


Figure A1.74. Job plots showing the relative integrations versus mole fractions of **11** (within the given ensemble) for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{8}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{11}$ (**B**) in 2.9 M DME/toluene at $-50\text{ }^\circ\text{C}$.

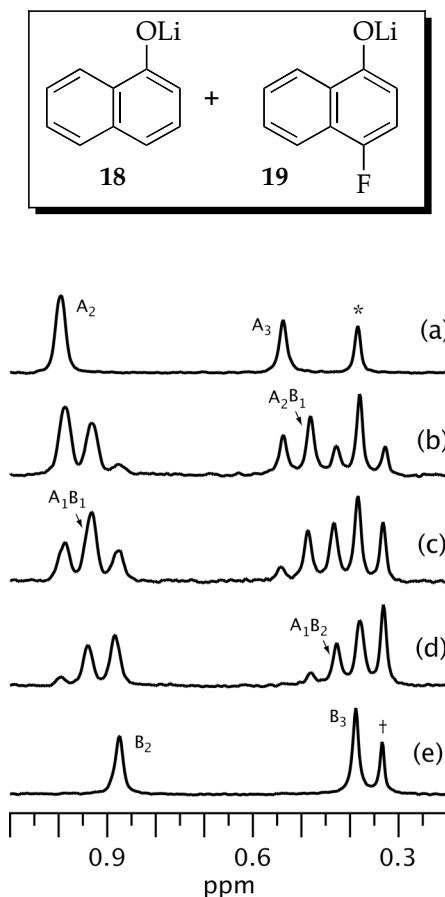


Figure A1.75. ^6Li NMR spectra of 0.10 M solutions of $[^6\text{Li}]\mathbf{18}$ (**A**) and $[^6\text{Li}]\mathbf{19}$ (**B**) at 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)–(e) are 0.00, 0.30, 0.49, 0.75, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate; † denotes **B**·LiHMDS mixed aggregate. Due to overlap of **B**₃ homoaggregate with **A**·LiHMDS mixed aggregate, the contribution to the peak's integration from **B**₃ was calculated as follows. Constant excess LiHMDS was assumed, therefore constant relative integration for **A**·LiHMDS + **B**·LiHMDS. Subtracting the measured **B**·LiHMDS integration from this for each tube gave a calculated **A**·LiHMDS integration, which was subtracted from the overlapped peak's integration to give a value for **B**₃.

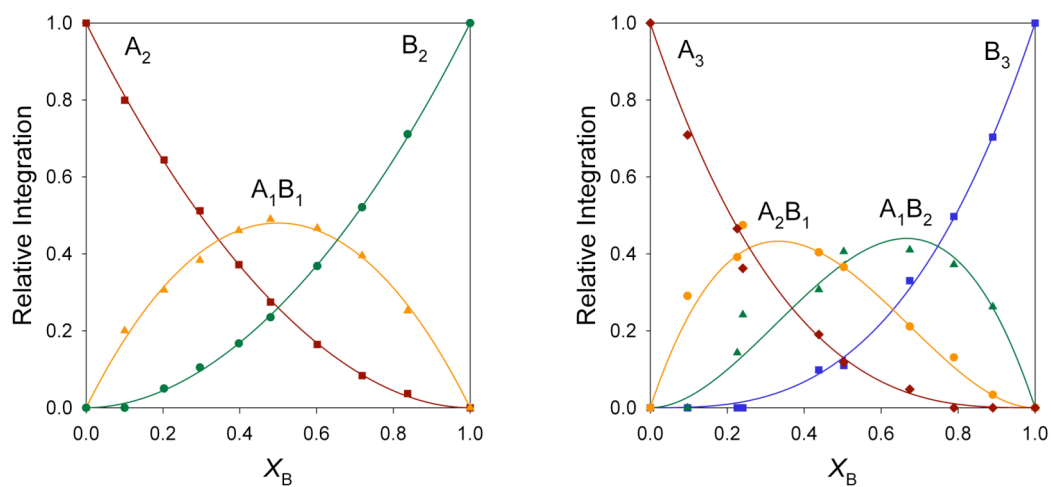
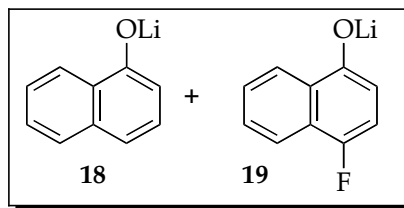


Figure A1.76. Job plots showing the relative integrations versus mole fractions of **19** (within the given ensemble) for 0.10 M mixtures of phenolates $[^6\text{Li}]\mathbf{18}$ (**A**) and $[^6\text{Li}]\mathbf{19}$ (**B**) in 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$.

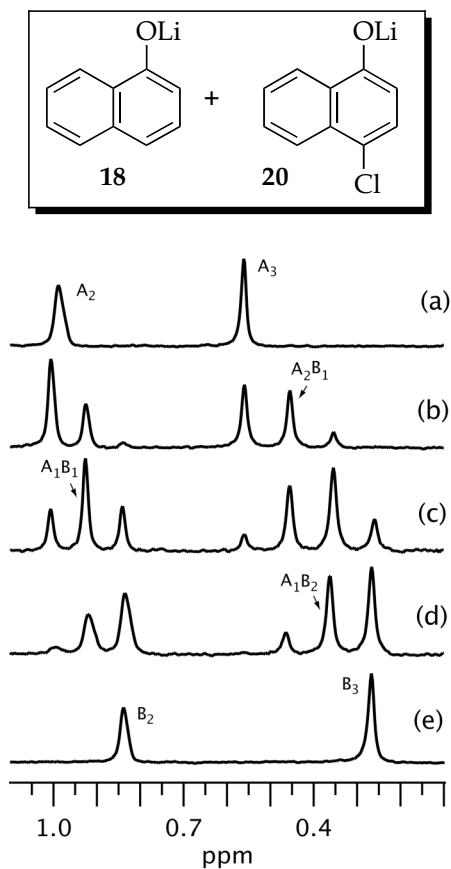


Figure A1.77. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{18}$ (A) and $[\text{}^6\text{Li}]\mathbf{20}$ (B) at 2.9 M DME/toluene at -90°C . The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.22, 0.54, 0.77, 1.00 respectively.

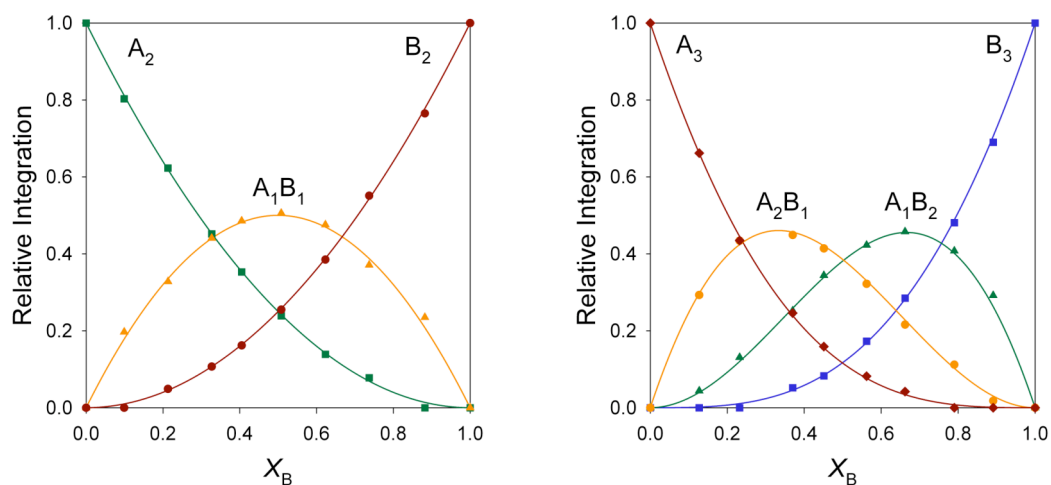


Figure A1.78. Job plots showing the relative integrations versus mole fractions of **20** (within the given ensemble) for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{18}$ (A) and $[\text{}^6\text{Li}]\mathbf{20}$ (B) in 2.9 M DME/toluene at -90°C .

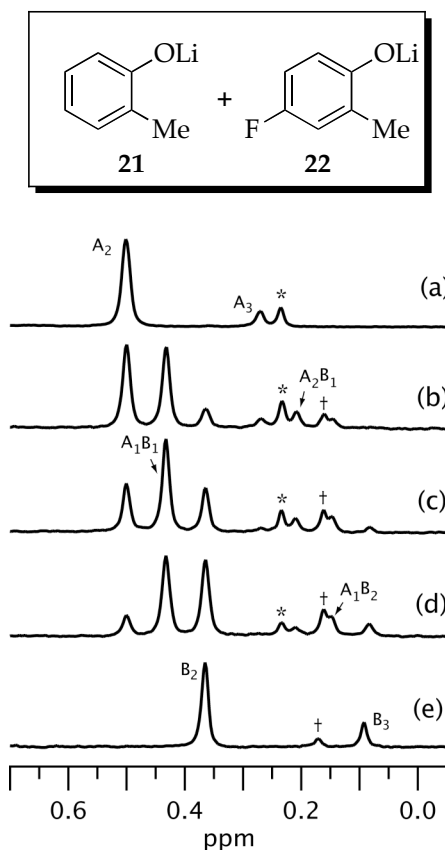


Figure A1.79. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{21}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{22}$ (**B**) at 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.33, 0.50, 0.66, 1.00 respectively. * denotes **A**·LiHMDS mixed aggregate; † denotes **B**·LiHMDS mixed aggregate.

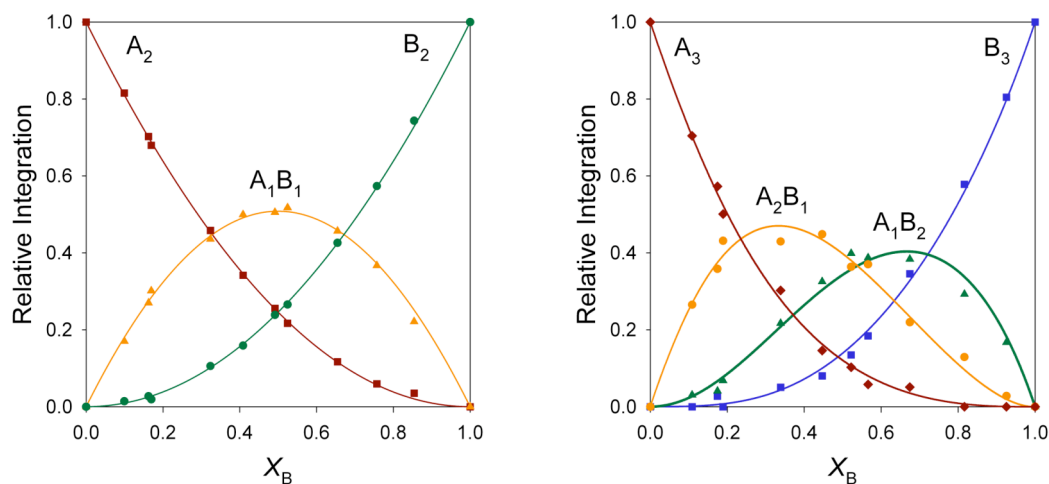


Figure A1.80. Job plots showing the relative integrations versus mole fractions of **22** (within the given ensemble) for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{21}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{22}$ (**B**) in 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$.

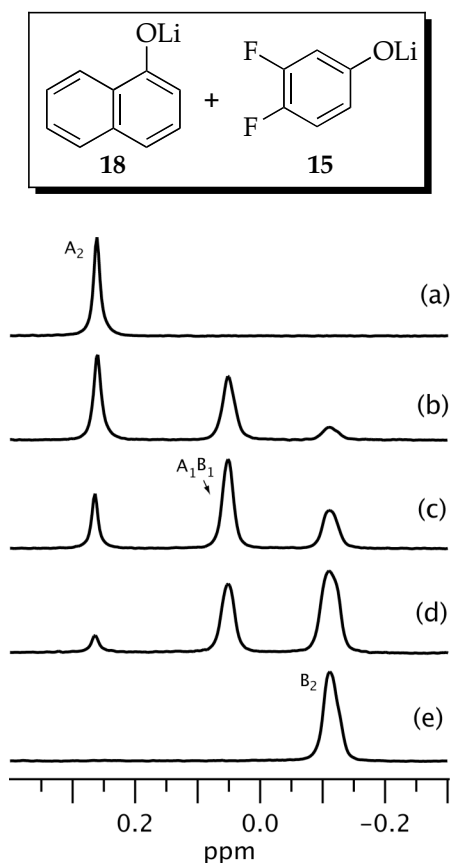


Figure A1.81. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{18}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{15}$ (**B**) at 0.22 M TMEDA/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.34, 0.53, 0.74, 1.00 respectively.

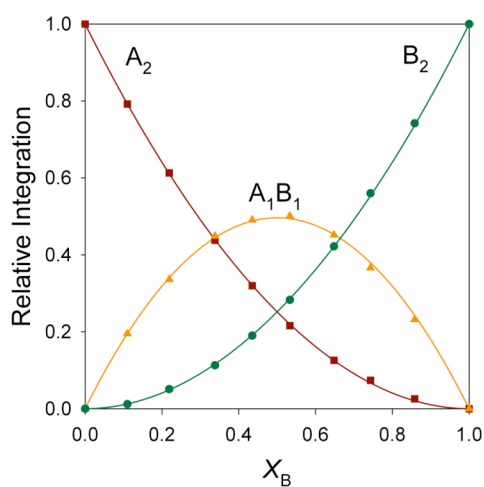


Figure A1.82. Job plot showing the relative integrations versus mole fractions of **15** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{18}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{15}$ (**B**) in 0.22 M TMEDA/toluene at $-90\text{ }^\circ\text{C}$.

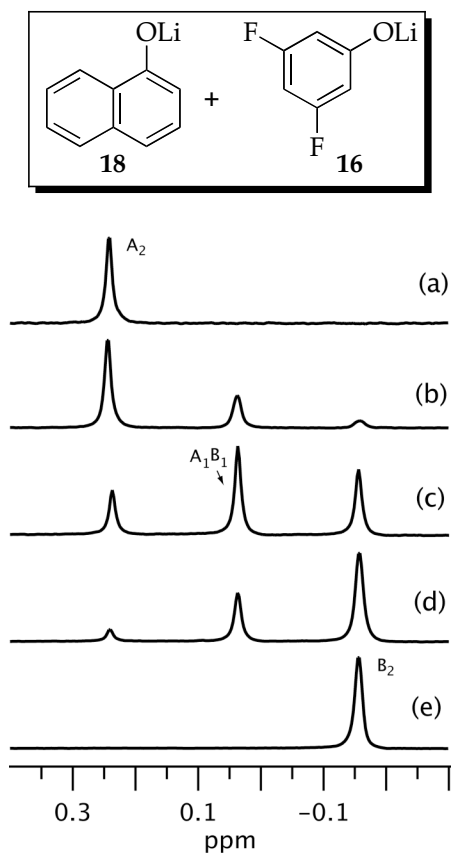


Figure A1.83. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{18}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{16}$ (**B**) at 0.22 M TMEDA/toluene at $-90\text{ }^\circ\text{C}$. The mole fractions of **B** in the tubes (a)-(e) are 0.00, 0.21, 0.55, 0.76, 1.00 respectively.

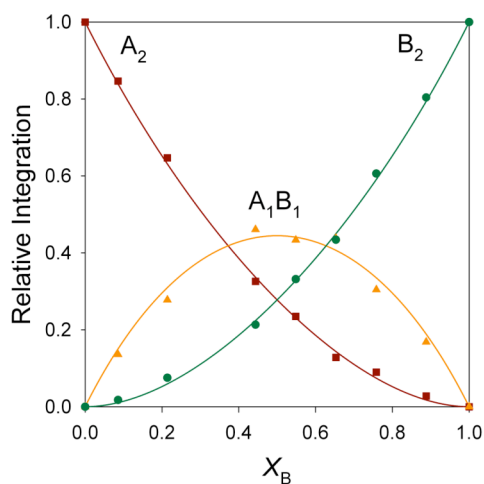


Figure A1.84. Job plot showing the relative integrations versus mole fractions of **16** for 0.10 M mixtures of phenolates $[\text{}^6\text{Li}]\mathbf{18}$ (**A**) and $[\text{}^6\text{Li}]\mathbf{16}$ (**B**) in 0.22 M TMEDA/toluene at $-90\text{ }^\circ\text{C}$.

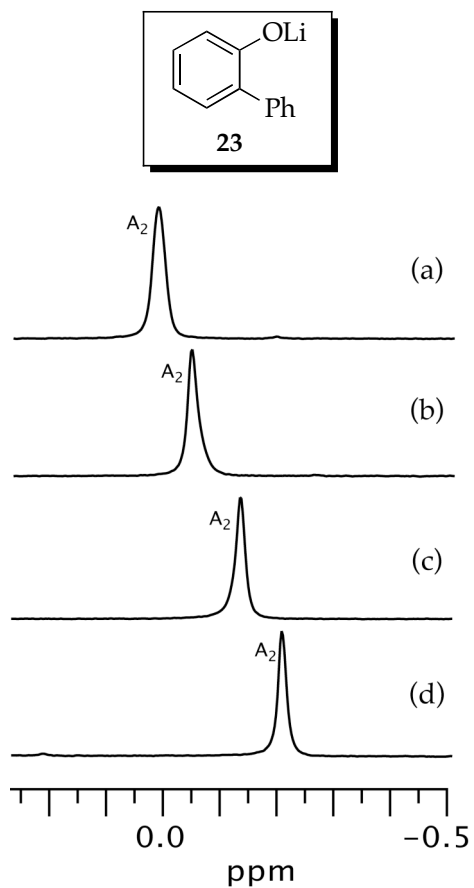


Figure A1.85. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{23}$ (**A**) at $-90\text{ }^\circ\text{C}$ showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 1.1 M THF/toluene in tube (d). Tubes (b) and (c) represent substitution of 11% and 50%, respectively, of the DME/toluene solvent with THF/toluene.

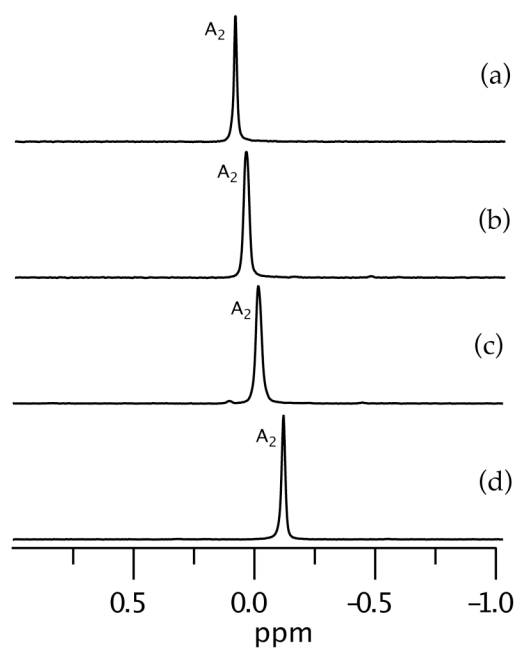
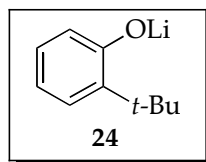


Figure A1.86. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{24}$ (**A**) at $-90\text{ }^\circ\text{C}$ showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 1.1 M THF/toluene in tube (d). Tubes (b) and (c) represent substitution of 11% and 50%, respectively, of the DME/toluene solvent with THF/toluene.

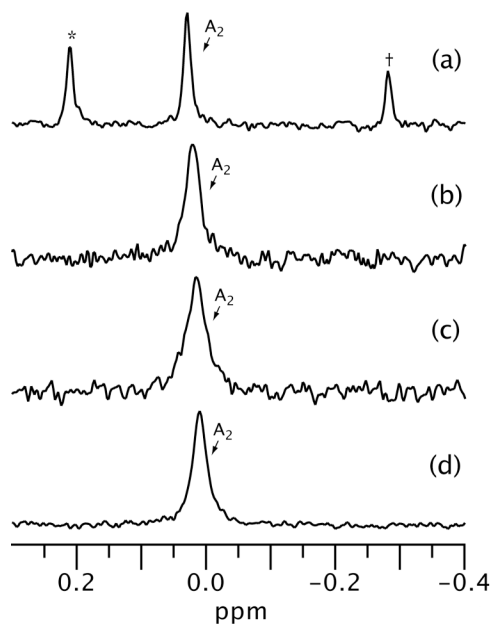
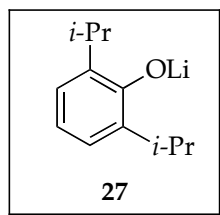


Figure A1.87. ^6Li NMR spectra of 0.10 M solutions of $[^6\text{Li}]\mathbf{27}$ (**A**) at $-90\text{ }^\circ\text{C}$ showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 1.1 M THF/toluene in tube (d). Tubes (b) and (c) represent substitution of 11% and 50%, respectively, of the DME/toluene solvent with THF/toluene. \dagger denotes excess LiHMDS dimer and $*$ denotes **A**.LiHMDS mixed aggregate.

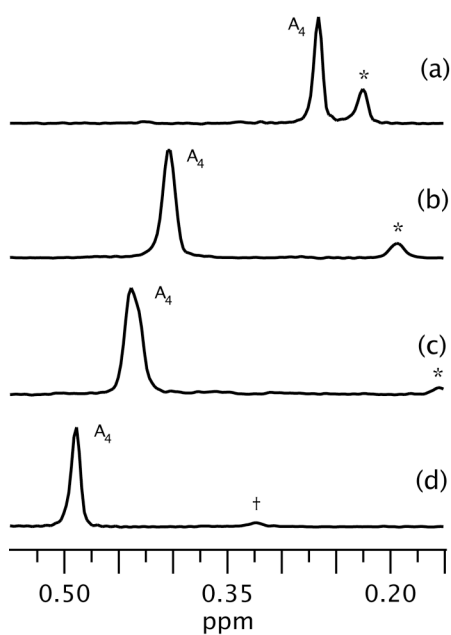
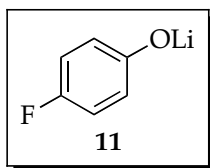


Figure A1.88. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{11}$ (**A**) at $-90\text{ }^\circ\text{C}$ showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 3.7 M THF/toluene in tube (d). Tubes (b) and (c) represent substitution of 17% and 33%, respectively, of the DME/toluene solvent with THF/toluene. * denotes $\mathbf{A}\cdot\text{LiHMDS}$ mixed aggregate; † denotes excess LiHMDS.

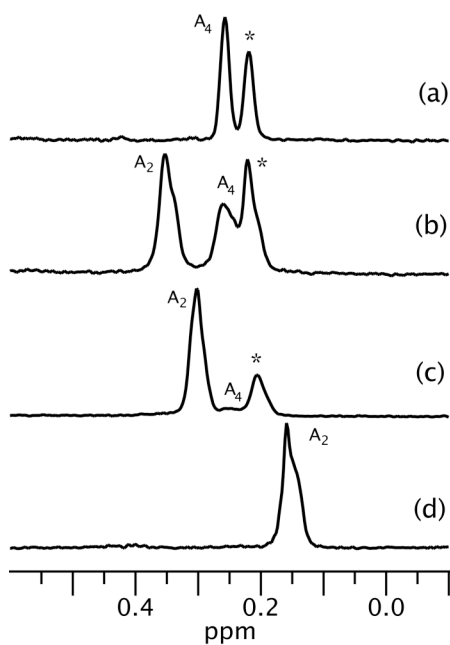
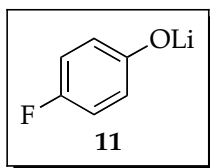


Figure A1.89. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{11}$ (**A**) at $-90\text{ }^\circ\text{C}$ showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 2.0 M TMEDA/toluene in tube (d). Tubes (b) and (c) represent substitution of 5% and 11%, respectively, of the DME/toluene solvent with TMEDA/toluene. * denotes $\mathbf{A}\cdot\text{LiHMDS}$ mixed aggregate.

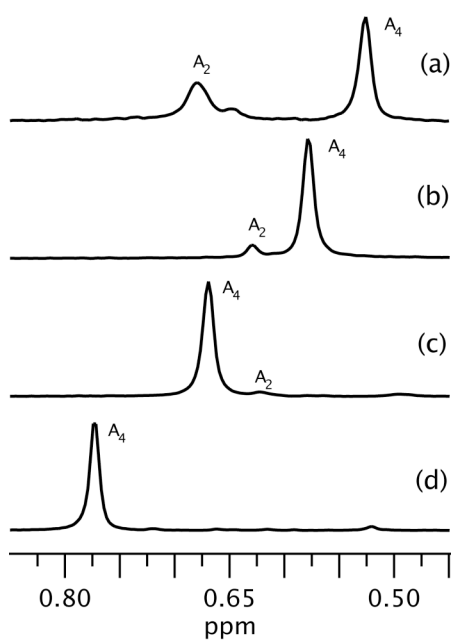
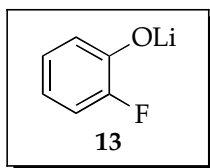


Figure A1.90. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{13}$ (**A**) at $-90\text{ }^\circ\text{C}$ showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 1.1 M THF/toluene in tube (d). Tubes (b) and (c) represent substitution of 11% and 33%, respectively, of the DME/toluene solvent with THF/toluene.

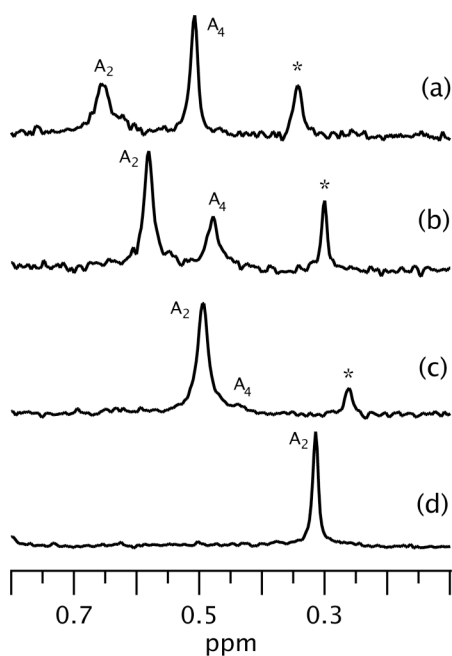
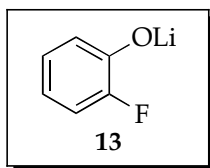


Figure A1.91. ^6Li NMR spectra of 0.10 M solutions of $[^6\text{Li}]\mathbf{13}$ (**A**) at $-90\text{ }^\circ\text{C}$ showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 0.22 M TMEDA/toluene in tube (d). Tubes (b) and (c) represent substitution of 11% and 33%, respectively, of the DME/toluene solvent with TMEDA/toluene. * denotes $\text{A}\cdot\text{LiHMDS}$ mixed aggregate.

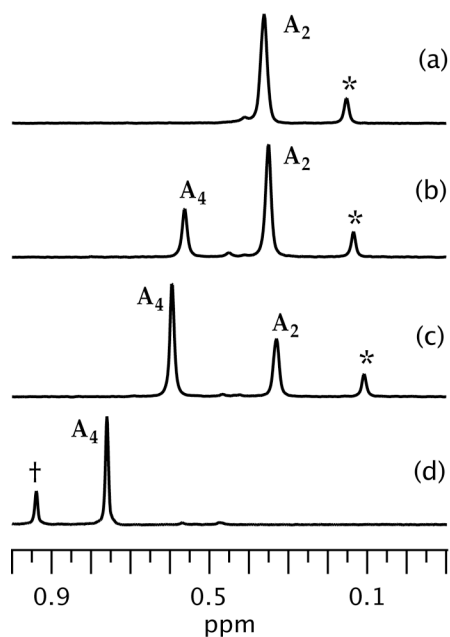
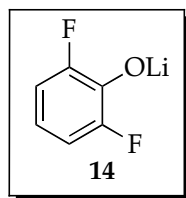


Figure A1.92. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{14}$ (**A**) at $-90\text{ }^\circ\text{C}$ showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 1.1 M THF/toluene in tube (d). Tubes (b) and (c) represent substitution of 17% and 33%, respectively, of the DME/toluene solvent with THF/toluene. * denotes $\mathbf{A}\cdot\text{LiHMDS}$ mixed aggregate; † denotes excess LiHMDS.

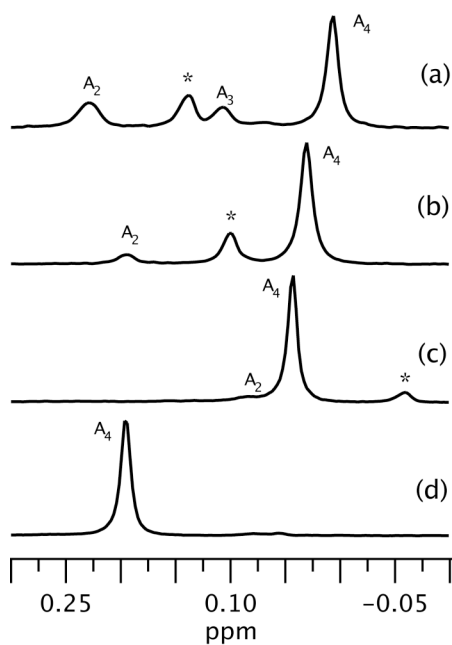
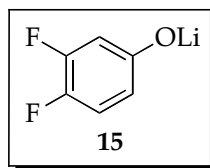


Figure A1.93. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{15}$ (**A**) at $-90\text{ }^\circ\text{C}$ showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 1.1 M THF/toluene in tube (d). Tubes (b) and (c) represent substitution of 17% and 72%, respectively, of the DME/toluene solvent with THF/toluene. * denotes $\mathbf{A}\cdot\text{LiHMDS}$ mixed aggregate.

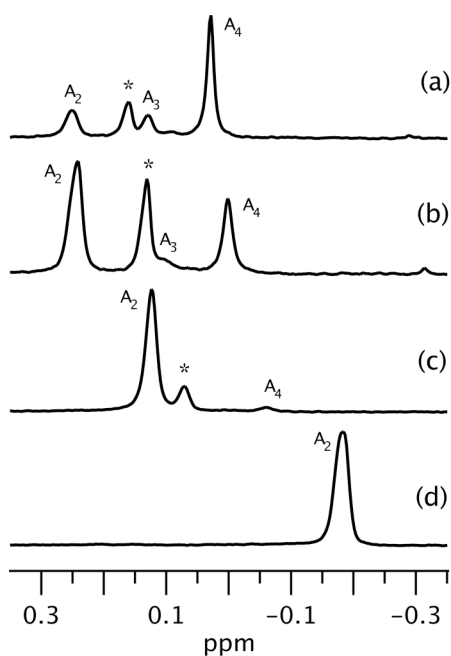
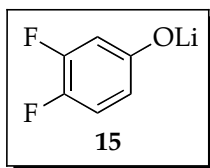


Figure A1.94. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{15}$ (**A**) at $-90\text{ }^\circ\text{C}$ showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 0.22 M TMEDA/toluene in tube (d). Tubes (b) and (c) represent substitution of 11% and 33%, respectively, of the DME/toluene solvent with TMEDA/toluene. * denotes $\text{A}\cdot\text{LiHMDS}$ mixed aggregate.

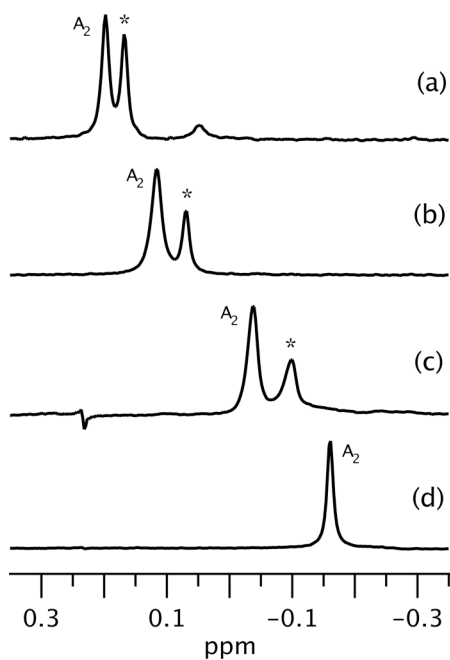
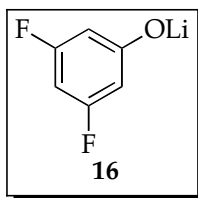


Figure A1.95. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{16}$ (**A**) at $-90\text{ }^\circ\text{C}$ showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 0.18 M TMEDA/toluene in tube (d). Tubes (b) and (c) represent substitution of 33% and 72%, respectively, of the DME/toluene solvent with TMEDA/toluene. * denotes $\mathbf{A}\cdot\text{LiHMDS}$ mixed aggregate.

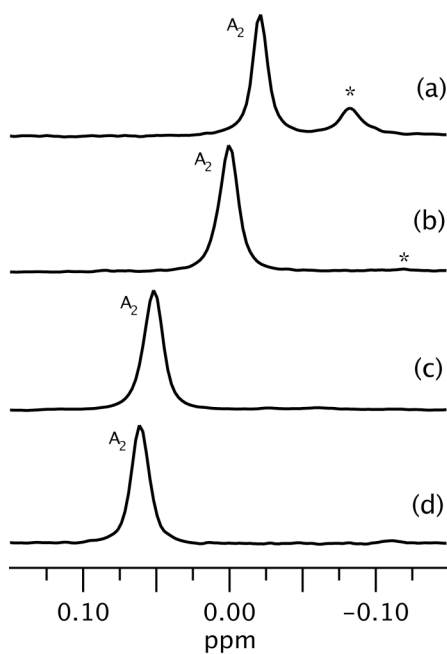
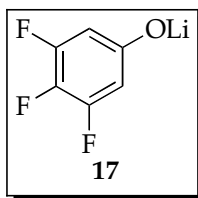


Figure A1.96. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{17}$ (**A**) at $-90\text{ }^\circ\text{C}$ showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 3.7 M THF/toluene in tube (d). Tubes (b) and (c) represent substitution of 22% and 50%, respectively, of the DME/toluene solvent with THF/toluene. * denotes $\mathbf{A}\cdot\text{LiHMDS}$ mixed aggregate.

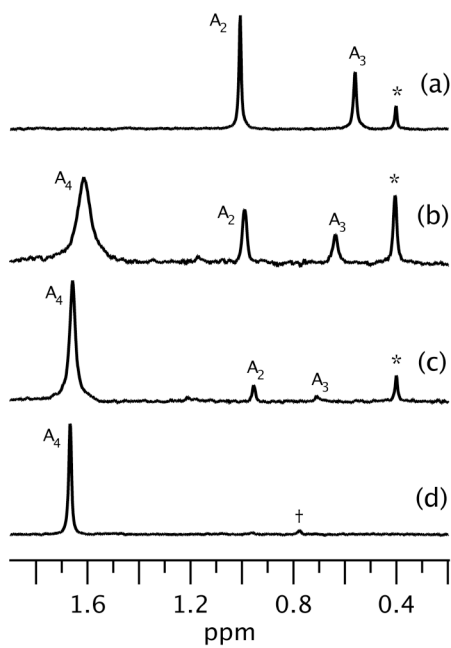
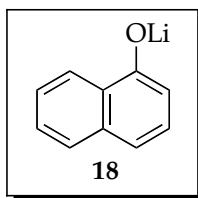


Figure A1.97. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{18}$ (**A**) at $-90\text{ }^\circ\text{C}$ showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 3.7 M THF/toluene in tube (d). Tubes (b) and (c) represent substitution of 6% and 11%, respectively, of the DME/toluene solvent with THF/toluene. * denotes $\mathbf{A}\cdot\text{LiHMDS}$ mixed aggregate; † denotes excess LiHMDS.

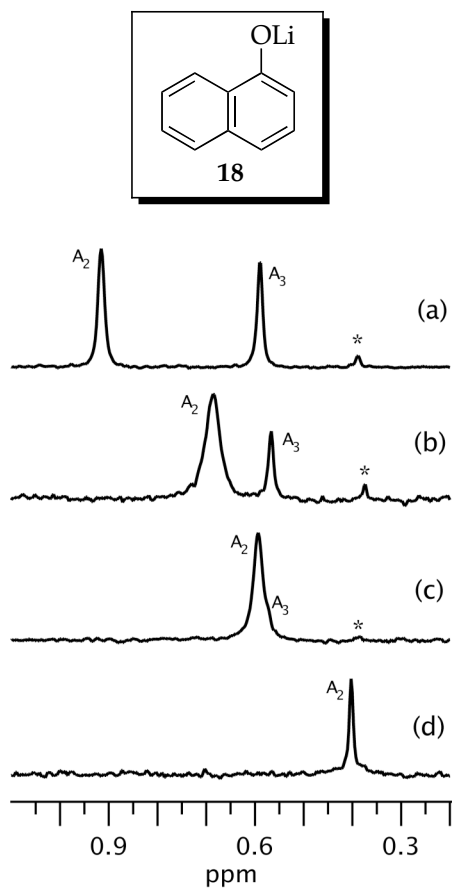


Figure A1.98. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{18}$ (**A**) at $-70\text{ }^\circ\text{C}$ showing a solvent substitution from 2.9 M DME/toluene in tube (a) to 2.0 M TMEDA/toluene in tube (d). Tubes (b) and (c) represent substitution of 3% and 6%, respectively, of the DME/toluene solvent with TMEDA/toluene. * denotes $\mathbf{A}\cdot\text{LiHMDS}$ mixed aggregate.

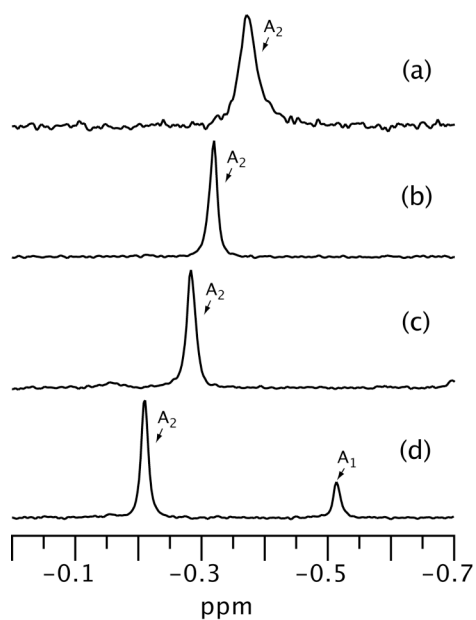
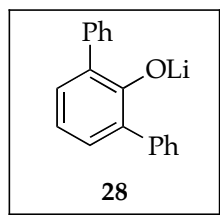


Figure A1.99. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{28}$ (**A**) at $-90\text{ }^\circ\text{C}$. The solvent systems in tubes (a)-(c) are 1.2 M, 2.0 M, 6.1 M THF/toluene, respectively; the solvent in tube (d) is neat THF (12.2 M). A_1 was tentatively assigned based on chemical shift similarity with other monomers.)

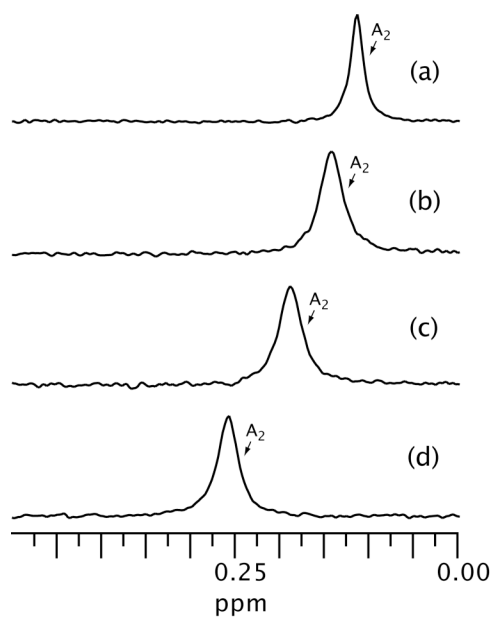
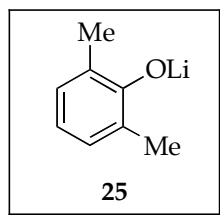


Figure A1.100. ^6Li NMR spectra of 0.10 M solutions of $[^6\text{Li}]\mathbf{25}$ (**A**) at $-90\text{ }^\circ\text{C}$. The solvent systems in tubes (a)-(d) are 2.0 M, 4.0 M, 6.1 M and 10.0 M THF/toluene, respectively.

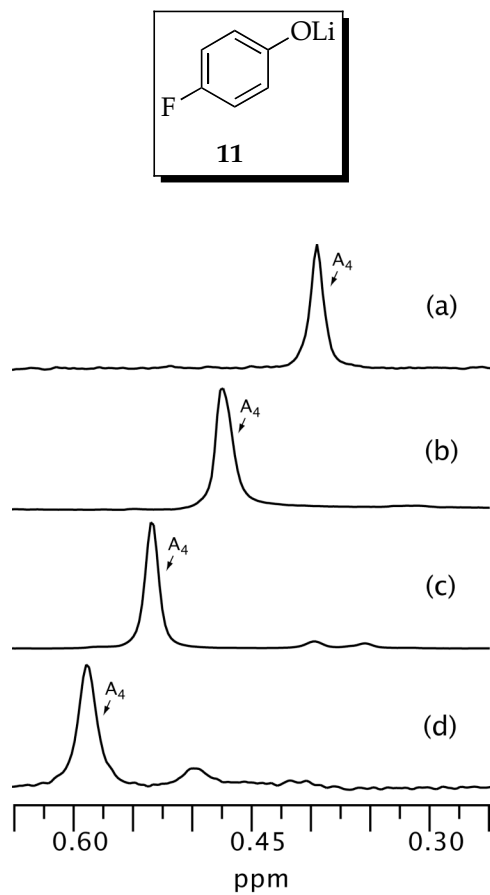


Figure A1.101. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{11}$ (**A**) at $-90\text{ }^\circ\text{C}$. The solvent systems in tubes (a)-(c) are 0.12 M, 2.0 M, 6.1 M THF/toluene, respectively; the solvent in tube (d) is neat THF (12.2 M).

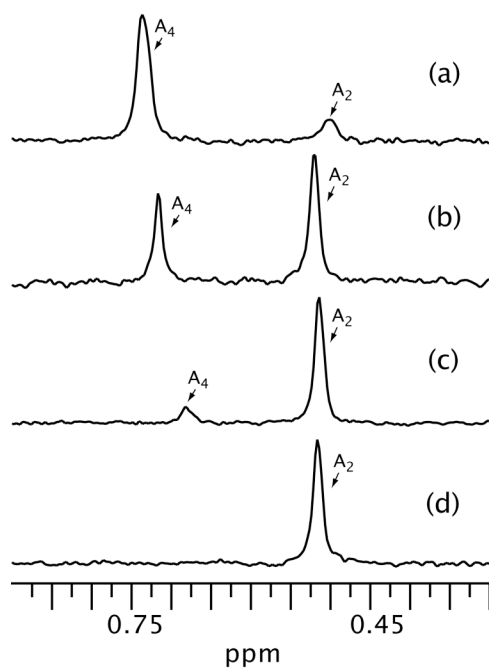
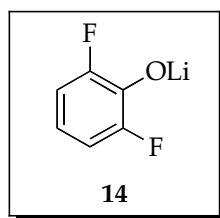


Figure A1.102. ^6Li NMR spectra of 0.10 M solutions of $[^6\text{Li}]\mathbf{14}$ (**A**) at $-90\text{ }^\circ\text{C}$. The solvent systems in tubes (a)-(d) are 2.0 M, 4.0 M, 6.1 M and 10.0 M THF/toluene, respectively. (A_2 was tentatively assigned based on chemical shift similarity with other dimers.)

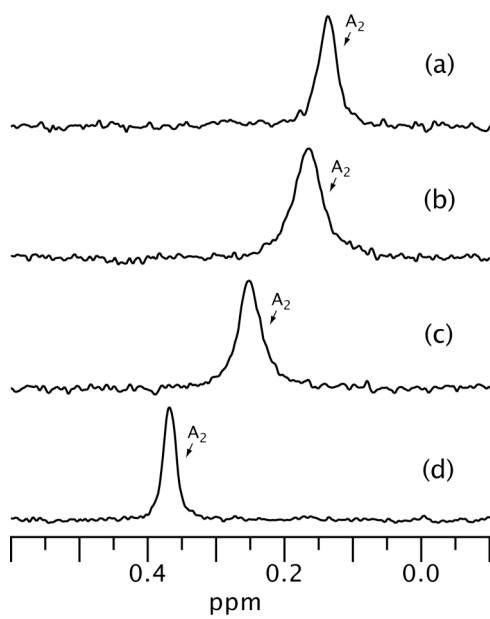
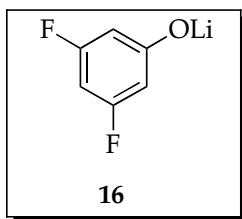


Figure A1.103. ^6Li NMR spectra of 0.10 M solutions of $[^6\text{Li}]\mathbf{16}$ (**A**) at $-90\text{ }^\circ\text{C}$. The solvent systems in tubes (a)-(d) are 2.0 M, 4.0 M, 6.1 M and 10.0 M THF/toluene, respectively.

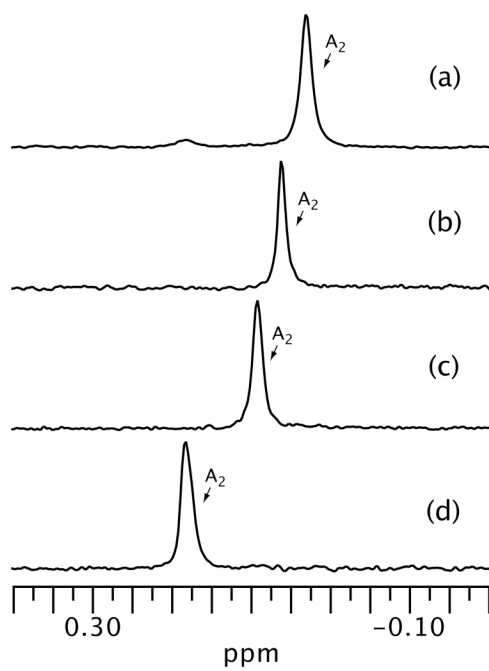
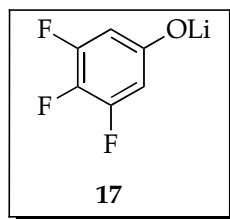


Figure A1.104. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{17}$ (**A**) at $-90\text{ }^\circ\text{C}$. The solvent systems in tubes (a)-(d) are 3.0 M, 4.0 M, 6.1 M and 8.0 M THF/toluene, respectively.

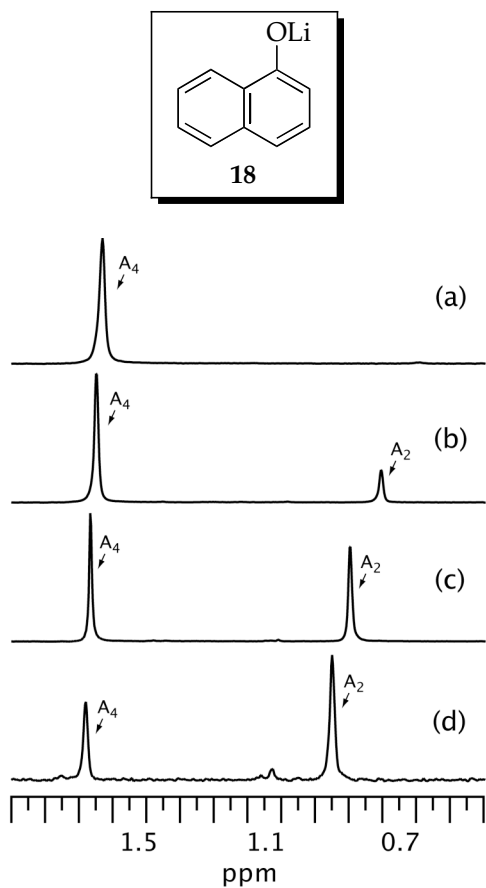


Figure A1.105. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{18}$ (**A**) at $-90\text{ }^\circ\text{C}$. The solvent systems in tubes (a)-(c) are 2.0 M, 6.0 M, 8.0 M THF/toluene, respectively; the solvent in tube (d) is neat THF (12.2 M).

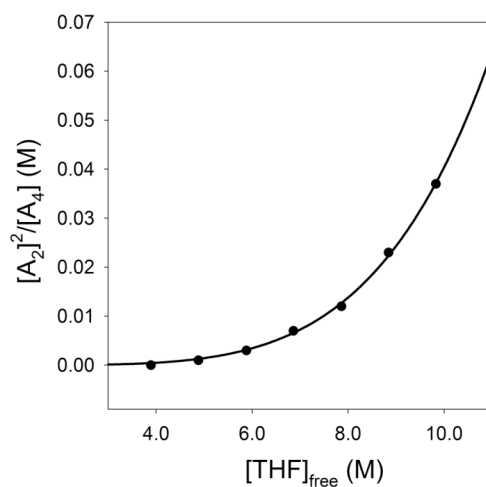
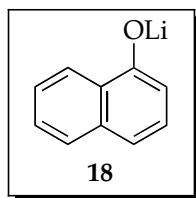
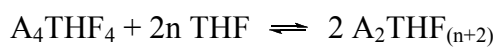


Figure A1.106. Plot of $[A_2]^2/[A_4]$ of 0.10 M [⁶Li]**8** (**A**) in toluene at -90 °C. The data are fit by non-linear least squares methods to the following power function ($K_{eq} = 6 \cdot 10^{-7} \pm 4 \cdot 10^{-7}$, $n = 2.4 \pm 0.3$) :

$$[A_2]^2/[A_4] = K_{eq} * [THF]^{2n}$$

The equation, assuming a tetrasolvated tetramer was derived from the following equilibrium:



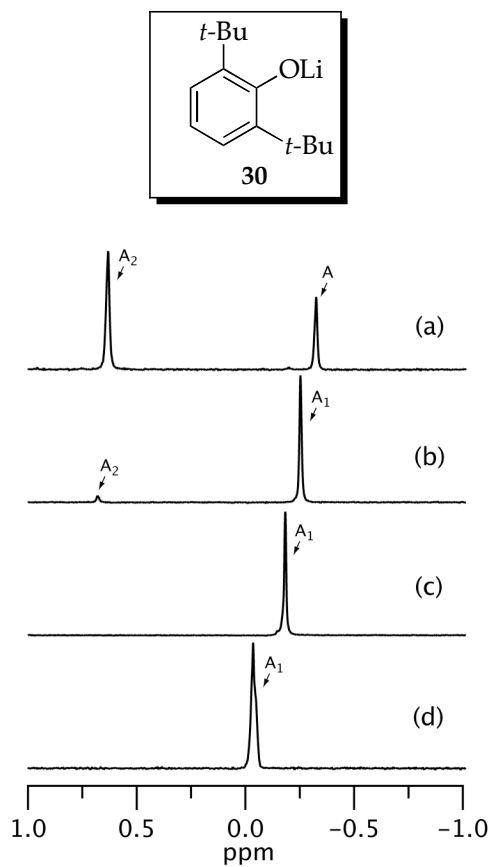


Figure A1.107. ^6Li NMR spectra of 0.10 M solutions of $[^6\text{Li}]\mathbf{30}$ (**A**) at $-90\text{ }^\circ\text{C}$. The solvent system in tubes (a)-(d) are 2.0 M, 4.0 M, 6.0 M, 10.0 M THF/toluene respectively.

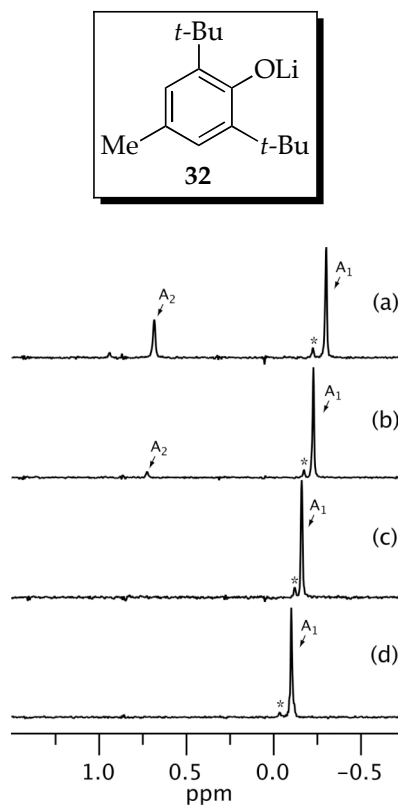


Figure A1.108. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{32}$ (**A**) at $-90\text{ }^\circ\text{C}$. The solvent systems in tubes (a)-(c) are 4.0 M, 6.0 M, 8.0 M THF/toluene, respectively; the solvent in tube (d) is neat THF (12.2 M).

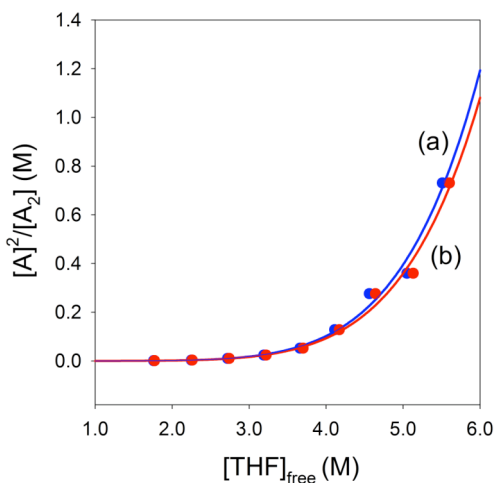
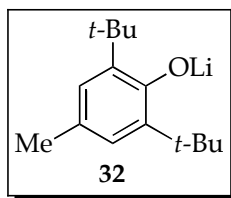


Figure A1.109. (a) Plot of $[A]^2/[A_2]$ of 0.10 M $[^6\text{Li}]\mathbf{32}$ (**A**) in toluene at $-90\text{ }^\circ\text{C}$. The data are fit by non-linear least squares methods to the following power function ($K_{\text{eq}} = 2 \cdot 10^{-5} \pm 3 \cdot 10^{-5}$, $n = 3.0 \pm 0.8$) :

$$[A]^2/[A_2] = K_{\text{eq}} * [\text{THF}]^{2n}$$

The equation, assuming a tetrasolvated dimer was derived from the following equilibrium:



(b) Plot of $[A]^2/[A_2]$ of 0.10 M $[^6\text{Li}]\mathbf{32}$ (**A**) in toluene at $-90\text{ }^\circ\text{C}$. The data are fit by non-linear least squares methods to the following power function ($K_{\text{eq}} = 2 \cdot 10^{-5} \pm 4 \cdot 10^{-5}$, $n = 3.0 \pm 0.9$) :

$$[A]^2/[A_2] = K_{\text{eq}} * [\text{THF}]^{2n}$$

The equation, assuming a disolvated dimer was derived from the following equilibrium:



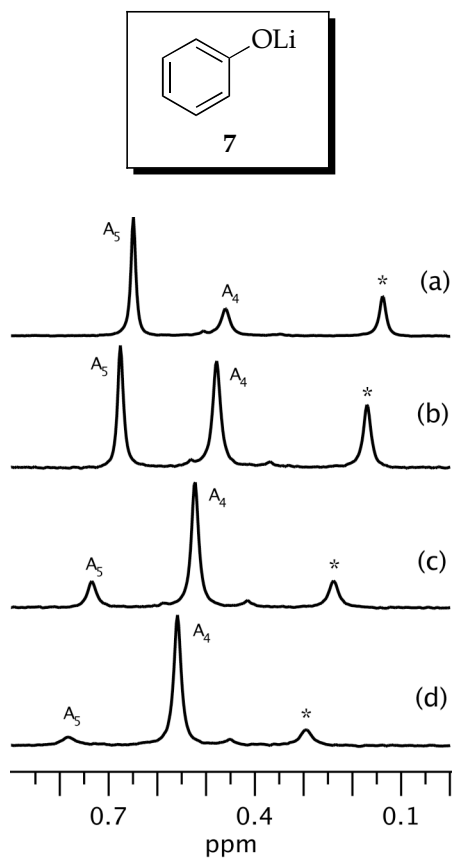


Figure A1.110. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{7}$ (**A**) at $-30\text{ }^\circ\text{C}$. The solvent systems in tubes (a)-(d) are 0.64 M, 1.1 M, 2.1 M and 2.9 M DME/toluene, respectively. * denotes $\mathbf{A}\cdot\text{LiHMDS}$ mixed aggregate.

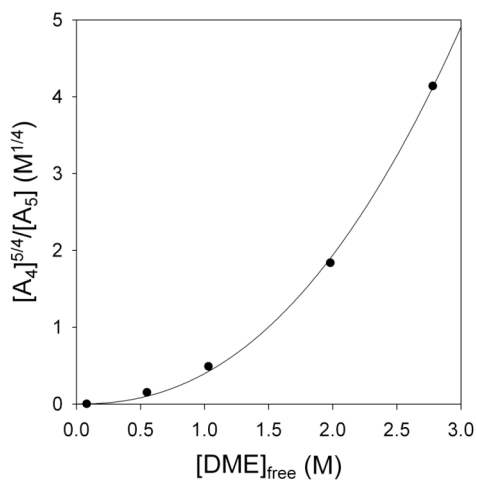
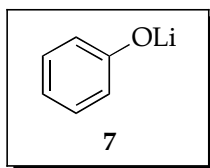


Figure A1.111. Plot of $[A_4]^{5/4}/[A_5]$ vs. $[DME]$ for 0.10 M $[^6Li]7$ (A) in toluene at $-30^\circ C$. The data are fit by non-linear least-squares methods to the following power function ($K_{eq} = 0.40 \pm 0.06$, $n = 2.7 \pm 0.2$):

$$[A_4]^{5/4}/[A_5] = K_{eq} * [DME]^{5-n}$$

The equation, assuming a tetrasolvated tetramer, was derived from the following equilibrium:



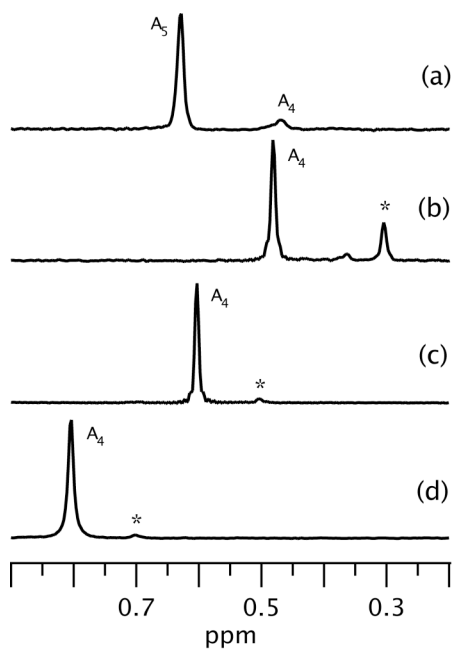
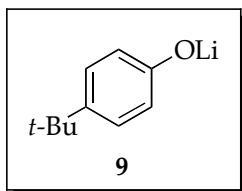


Figure A1.112. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{9}$ (**A**) at $-90\text{ }^\circ\text{C}$ (tube (a) at $-30\text{ }^\circ\text{C}$, tube (d) at $-70\text{ }^\circ\text{C}$). The solvent systems in tubes (a)-(c) are 0.24 M, 2.9 M and 6.3 M DME/toluene, respectively; the solvent in tube (d) is neat DME (9.6 M). * denotes $\mathbf{A}\cdot\text{LiHMDS}$ mixed aggregate.

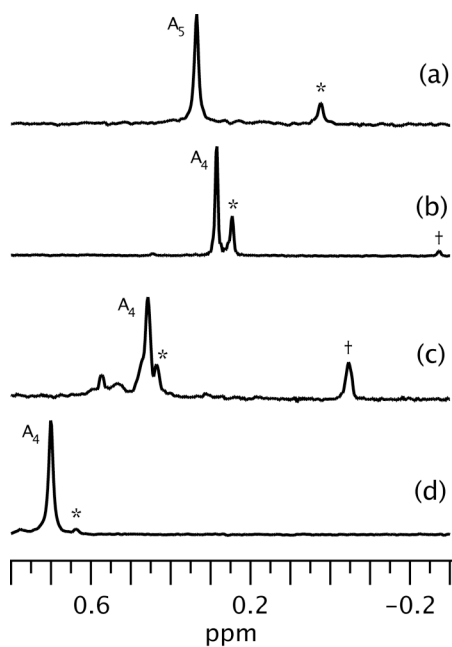
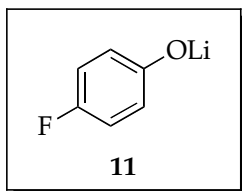


Figure A1.113. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{11}$ (**A**) at $-90\text{ }^\circ\text{C}$ (tube (a) at $-30\text{ }^\circ\text{C}$, tube (d) at $-70\text{ }^\circ\text{C}$). The solvent systems in tubes (a)-(c) are 0.22 M, 2.9 M and 6.3 M DME/toluene, respectively; the solvent in tube (d) is neat DME (9.6 M). * denotes **A**·LiHMDS mixed aggregate; † denotes excess LiHMDS.

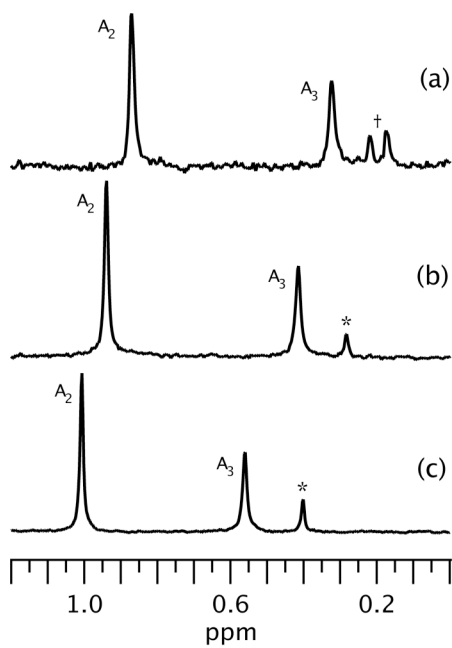
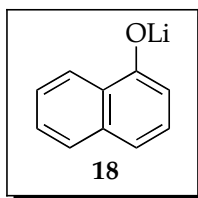


Figure A1.114. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{18}$ (**A**) at $-90\text{ }^\circ\text{C}$. The solvent systems in tubes (a)-(c) are 0.23 M, 1.1 M and 2.9 M DME/toluene, respectively. * denotes $\mathbf{A}\cdot\text{LiHMDS}$ mixed aggregate; † denotes $[\text{}^6\text{Li}, \text{}^{15}\text{N}]\mathbf{A}\cdot\text{LiHMDS}$ mixed aggregate.

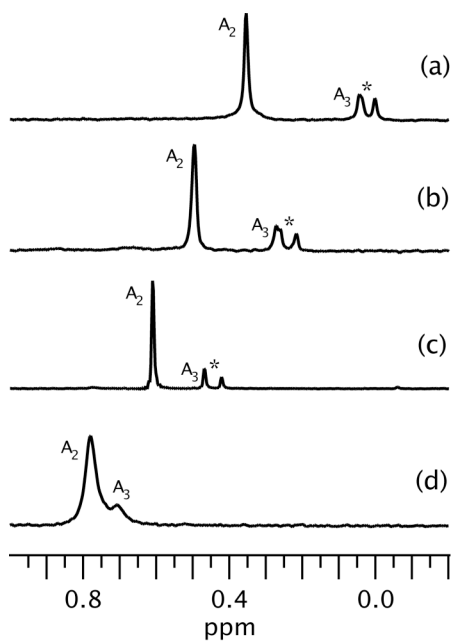
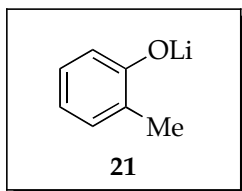


Figure A1.115. ^6Li NMR spectra of 0.10 M solutions of $[^6\text{Li}]\mathbf{21}$ (**A**) at $-90\text{ }^\circ\text{C}$ (tube (d) at $-70\text{ }^\circ\text{C}$). The solvent systems in tubes (a)-(c) are 0.24 M, 2.9 M and 6.3 M DME/toluene, respectively; the solvent in tube (d) is neat DME (9.6 M). * denotes $[^6\text{Li}, ^{15}\text{N}]\mathbf{A}\cdot\text{LiHMDS}$ mixed aggregate, half of which overlaps the A_3 peak.

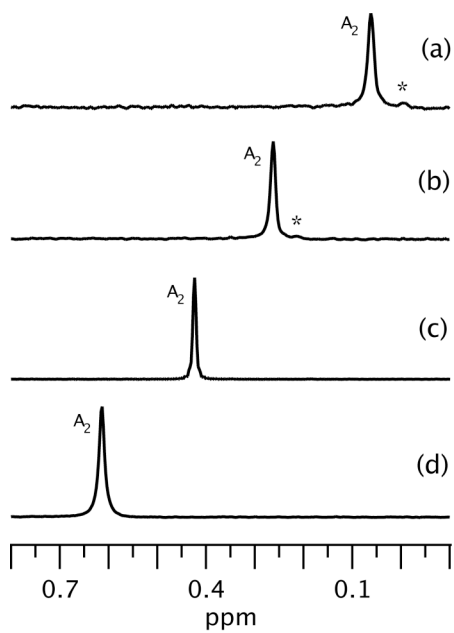
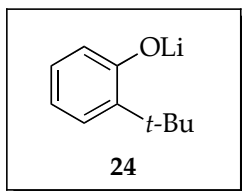


Figure A1.116. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{24}$ (**A**) at $-90\text{ }^\circ\text{C}$ (tube (d) at $-70\text{ }^\circ\text{C}$). The solvent systems in tubes (a)-(c) are 0.24 M, 2.9 M and 6.3 M DME/toluene, respectively; the solvent in tube (d) is neat DME (9.6 M). * denotes **A**·LiHMDS mixed aggregate.

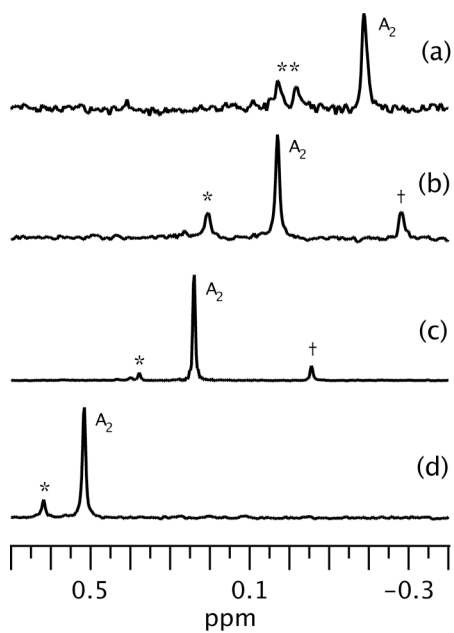
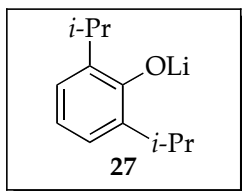


Figure A1.117. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{27}$ (**A**) at $-90\text{ }^\circ\text{C}$ (tube (d) at $-70\text{ }^\circ\text{C}$). The solvent systems in tubes (a)-(c) are 0.24 M, 2.9 M and 6.3 M DME/toluene, respectively; the solvent in tube (d) is neat DME (9.6 M). * denotes $\mathbf{A}\cdot\text{LiHMDS}$ mixed aggregate; ** denotes $[\text{}^6\text{Li}, \text{}^{15}\text{N}]\mathbf{A}\cdot\text{LiHMDS}$ mixed aggregate; † denotes excess LiHMDS.

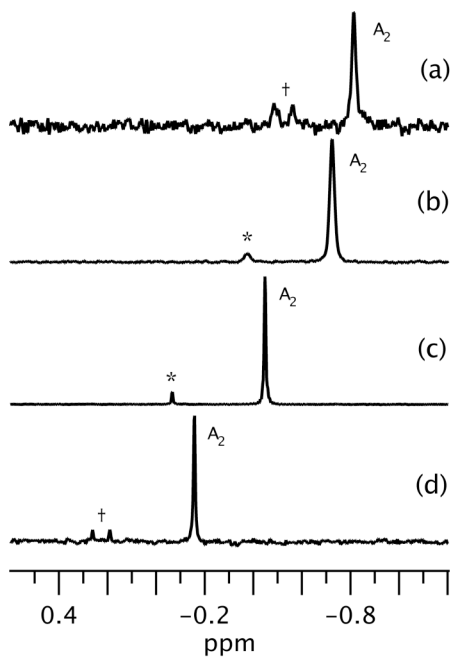
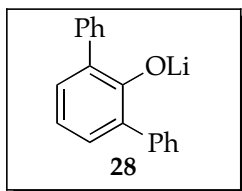


Figure A1.118. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{28}$ (A) at $-90\text{ }^\circ\text{C}$ (tube (d) at $-70\text{ }^\circ\text{C}$). The solvent systems in tubes (a)-(c) are 0.24 M, 2.9 M and 6.3 M DME/toluene, respectively; the solvent in tube (d) is neat DME (9.6 M). * denotes excess LiHMDS; † denotes excess $[\text{}^6\text{Li}, \text{}^{15}\text{N}]\text{LiHMDS}$.

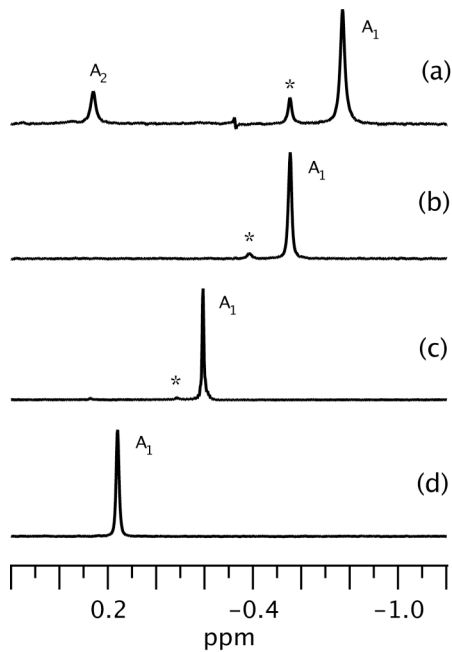
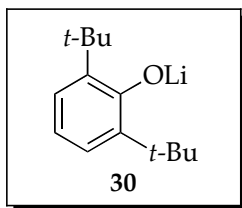


Figure A1.119. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{24}$ (**A**) at $-90\text{ }^\circ\text{C}$ (tube (d) at $-70\text{ }^\circ\text{C}$). The solvent systems in tubes (a)-(c) are 0.21 M, 2.9 M and 6.3 M DME/toluene, respectively; the solvent in tube (d) is neat DME (9.6 M). * denotes excess LiHMDS.

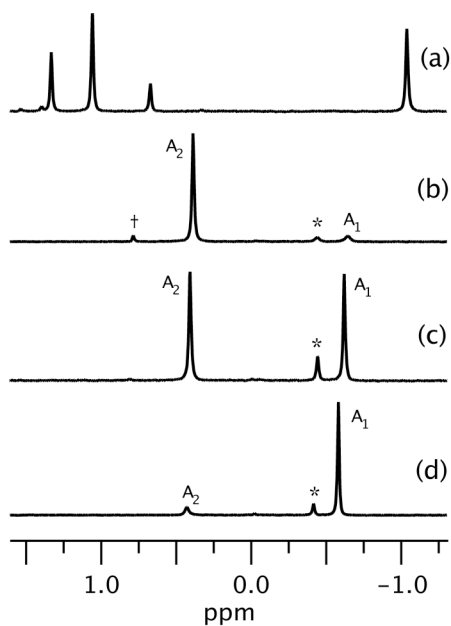
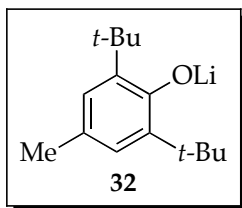


Figure A1.120. ^6Li NMR spectra of 0.10 M solutions of $[\text{}^6\text{Li}]\mathbf{32}$ (**A**) at $-70\text{ }^\circ\text{C}$. The solvent in tube (a) is toluene without added DME; the peaks have not been assigned. The solvent systems in tubes (b)-(d) are 0.22 M, 0.43 M and 0.87 M DME/toluene, respectively. * denotes excess LiHMDS monomer; † denotes LiHMDS dimer.

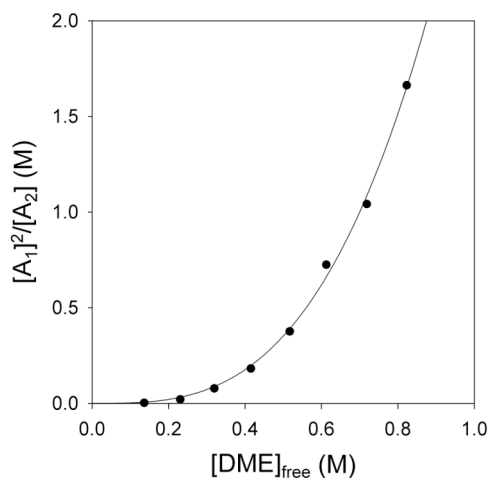
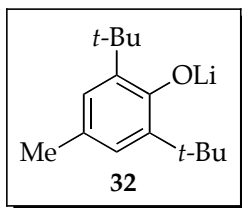


Figure A1.121. Plot of $[A_1]^2/[A_2]$ vs. $[DME]$ for 0.10 M $[^6Li]32$ (**A**) in toluene at -70 °C. The data are fit by non-linear least squares methods to the following power function ($K_{eq} = 3.0 \pm 0.2$, $n = 1.6 \pm 0.1$):

$$[A_1]^2/[A_2] = K_{eq} * [DME]^{2n}$$

The equation, assuming a monosolvated dimer, was derived from the following equilibrium:



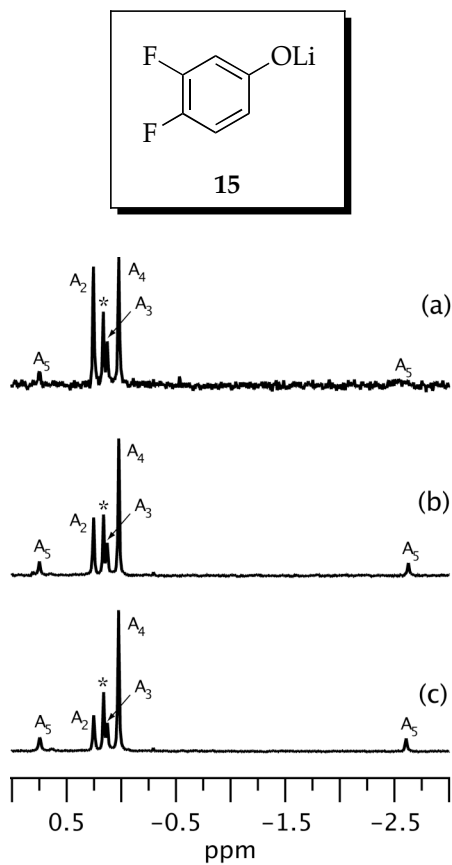


Figure A1.122. ^6Li NMR spectra of solutions of $[^6\text{Li}]\mathbf{15}$ (**A**) at 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$. The total lithium ion concentrations in tubes (a) – (c) are 0.018 N, 0.055 N and 0.109 N, respectively. * denotes excess LiHMDS.

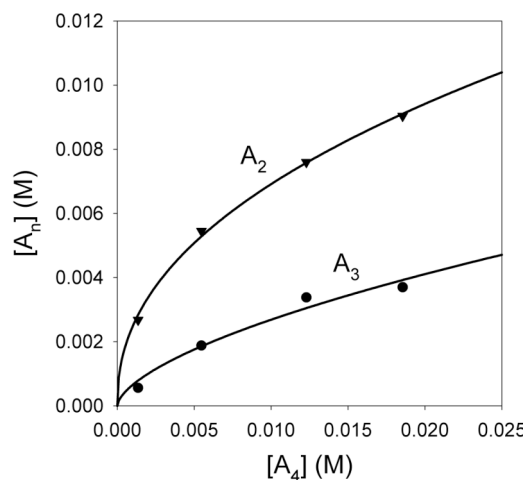
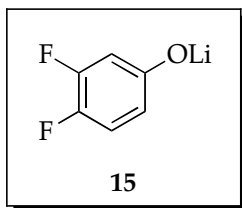
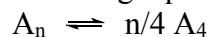


Figure A1.123. Plots of $[A_2]$ vs. $[A_4]$ and $[A_3]$ vs. $[A_4]$ for $[^6\text{Li}]\mathbf{15}$ (**A**) in 2.9 M DME/toluene at $-90\text{ }^\circ\text{C}$. The data are fit by non-linear least-squares methods to the following power function (A_2 : $K_{\text{eq}} = 19 \pm 2$, $n = 1.8 \pm 0.1$; A_3 : $K_{\text{eq}} = 22 \pm 7$, $n = 2.5 \pm 0.5$):

$$[A_n] = K_{\text{eq}}^{-1} * [A_4]^{n/4}$$

The equation was derived from the following equilibrium:



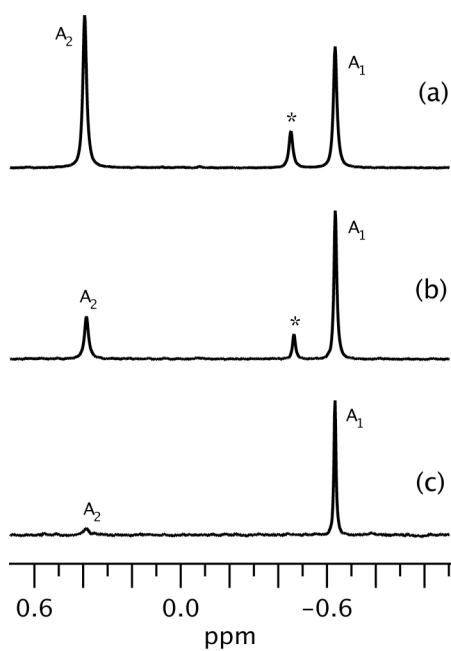
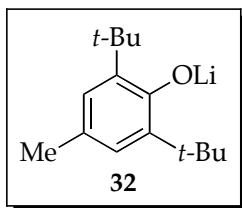


Figure A1.124. ^6Li NMR spectra of solutions of $[\text{}^6\text{Li}]\mathbf{32}$ (**A**) at cA. 0.4 M excess DME/toluene at $-70\text{ }^\circ\text{C}$. The total lithium ion concentrations in tubes (a) – (c) are 0.229 N, 0.057 N and 0.011 N, respectively. * denotes excess LiHMDS.

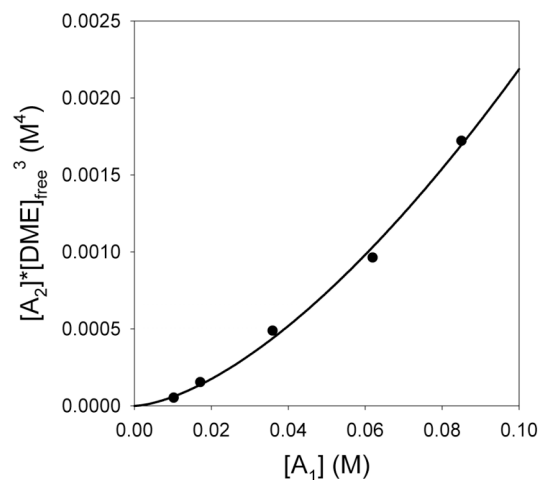
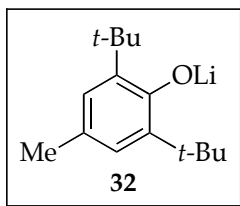
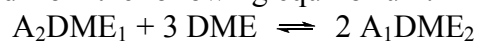


Figure A1.125. Plot of $[A_2]*[DME]_{\text{free}}^3$ vs. $[A_1]$ for $[^6\text{Li}]\mathbf{32}$ (**A**) in cA. 0.4 M excess DME/toluene at -70 °C. The data are fit by non-linear least-squares methods to the following power function ($K_{\text{eq}} = 12 \pm 3$, $n = 1.6 \pm 0.1$):

$$[A_2]*[DME]_{\text{free}}^3 = K_{\text{eq}}^{-1} * [A_1]^n$$

The equation was derived from the following equilibrium:



VI. ^{19}F NMR spectra.

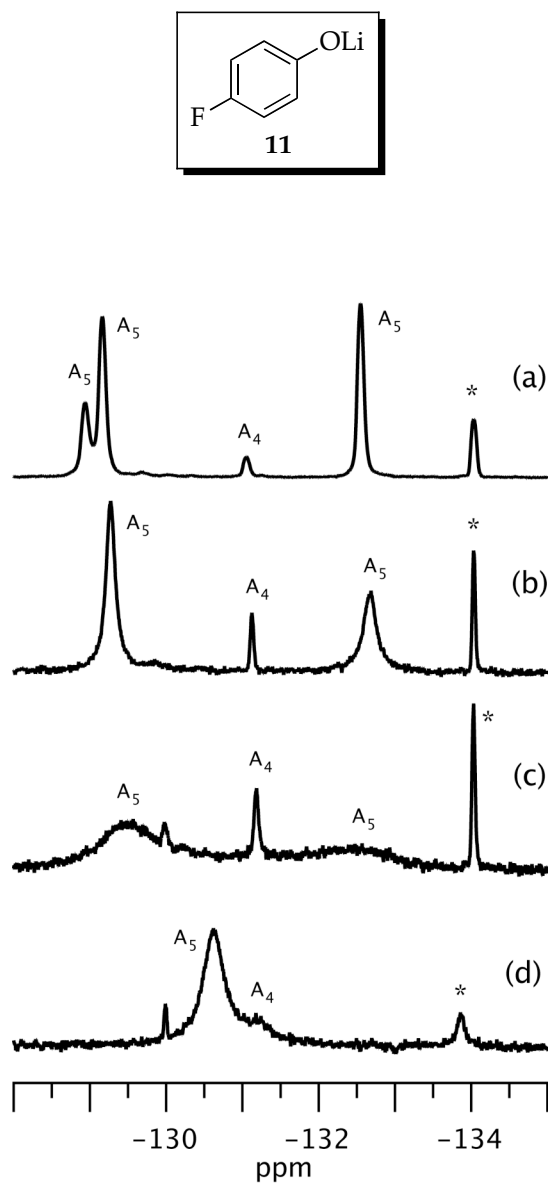


Figure A1.126. ^{19}F NMR spectra of a 0.10 M solution of **11** (**A**) in 0.22 M DME/toluene at (a) -90 °C, (b) -40 °C, (c) -20 °C, and (d) 10 °C. * denotes $\text{A} \cdot \text{LiHMDS}$ mixed aggregate.

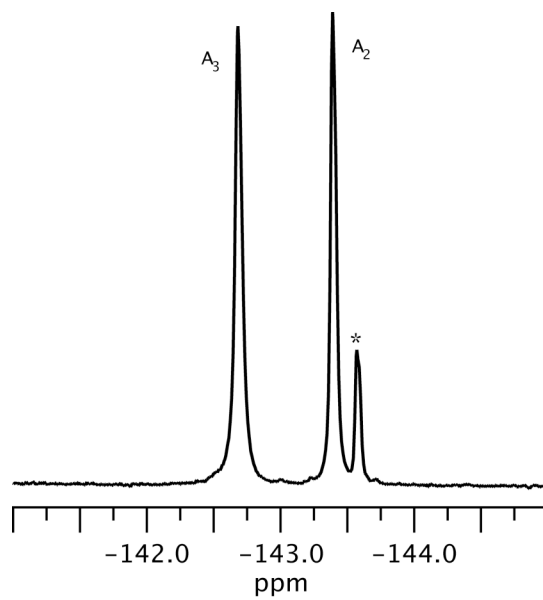
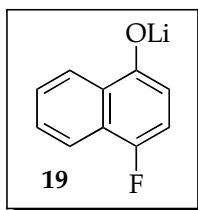


Figure A1.127. ^{19}F NMR spectrum of a 0.10 M solution of **19** (**A**) in 2.9 M DME/toluene at $-90\text{ }^{\circ}\text{C}$. * denotes A·LiHMDS mixed aggregate.

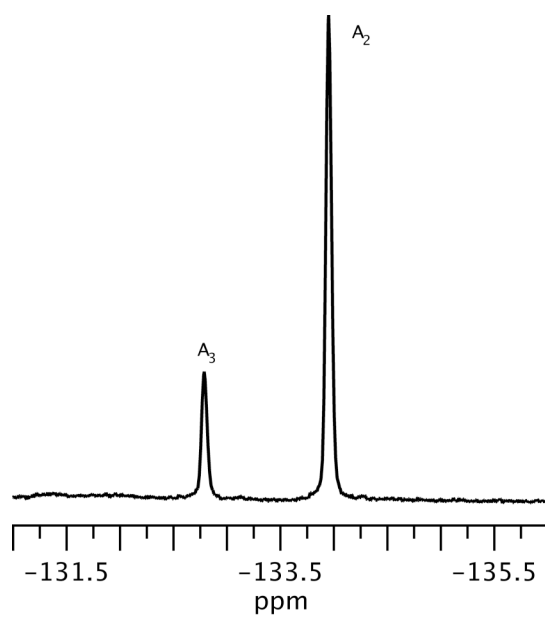
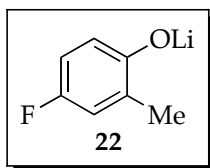


Figure A1.128. ^{19}F NMR spectrum of a 0.10 M solution of **22** (**A**) in 2.9 M DME/toluene at $-90\text{ }^{\circ}\text{C}$.

VI. Computational Studies.

Scheme 1.2. Equilibria among different aggregation states in DME and Me₂O

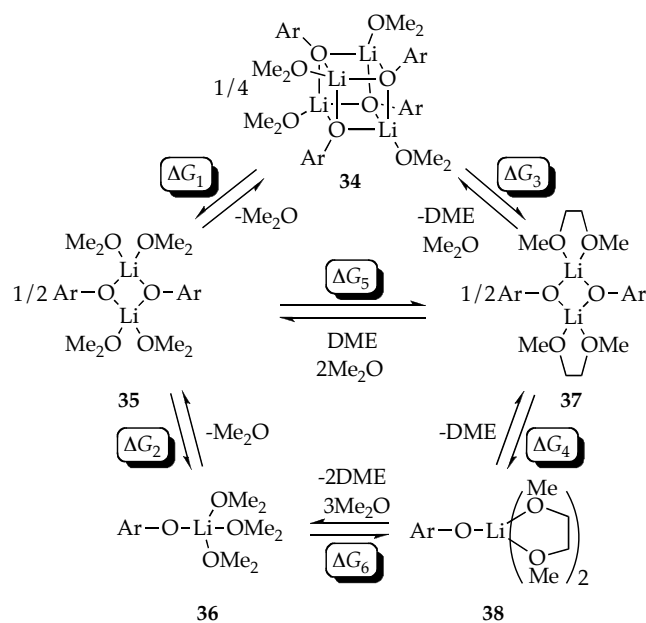
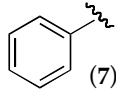
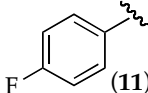
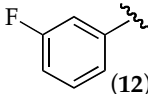
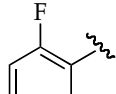
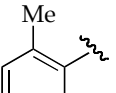
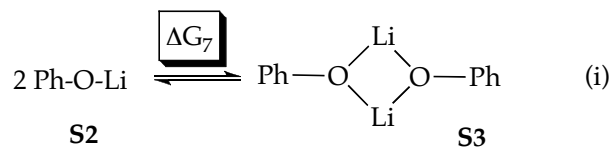


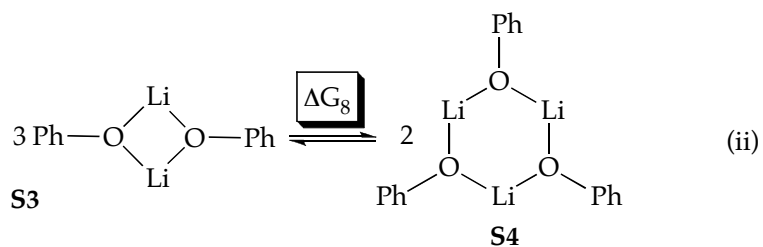
Table 1.3. Free energies ΔG_1 - ΔG_6 reported in kcal/mol on a per-lithium basis. The signs correspond to the affiliated arrows in Scheme 1.2.

-Ar (#)	ΔG_1	ΔG_2	ΔG_3	ΔG_4	ΔG_5	ΔG_6
 (7)	3.67	10.43	-0.11	10.05	-3.78	-4.16
 (11)	3.79	9.86	-0.14	10.23	-3.92	-4.29
 (12)	3.27	10.59	-0.03	8.98	-3.30	-4.91
 (13)	3.80	9.25	-0.36	7.21	-3.47	-5.51
 (25)	0.21	6.75	-6.22	10.06	-6.40	-3.12

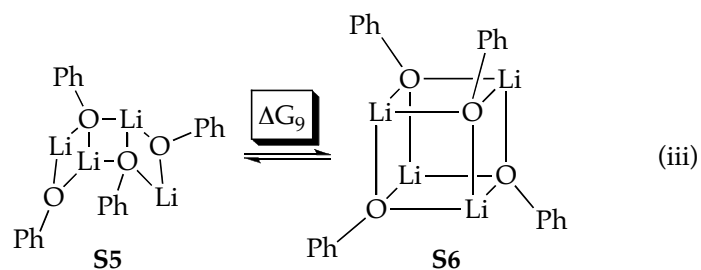
Unsolvated aggregates: Phenolate as a model system



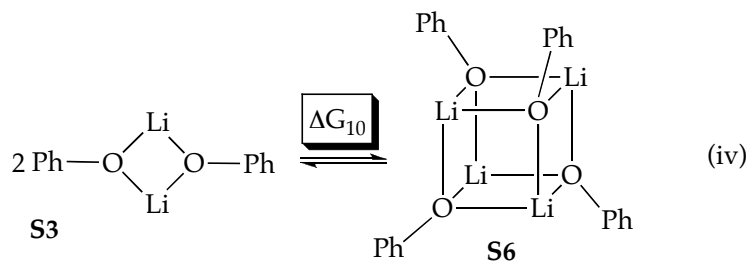
$$\Delta G_7 = -25.87 \text{ kcal/mol}$$



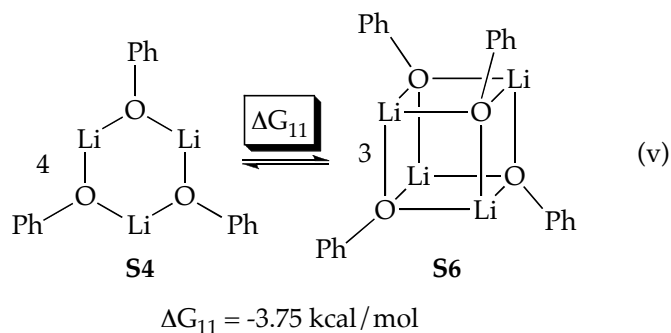
$$\Delta G_8 = -6.39 \text{ kcal/mol}$$



$$\Delta G_9 = -3.03 \text{ kcal/mol}$$



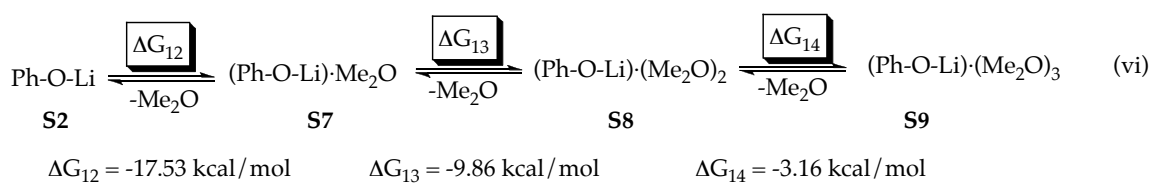
$$\Delta G_{10} = -10.14 \text{ kcal/mol}$$



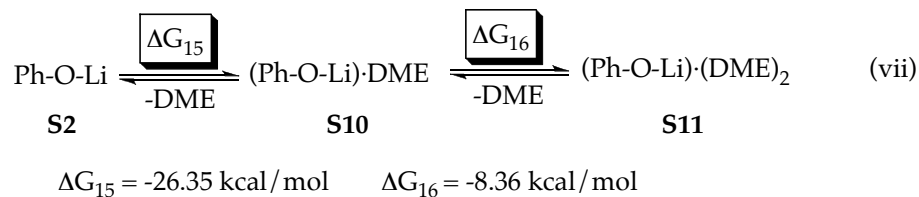
Serial solvation within same aggregates: Phenolate as a model system

Monomer solvation

S=Me₂O

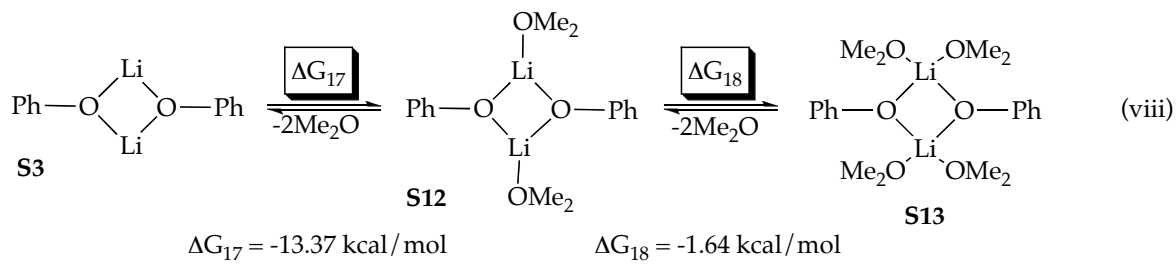


S=DME

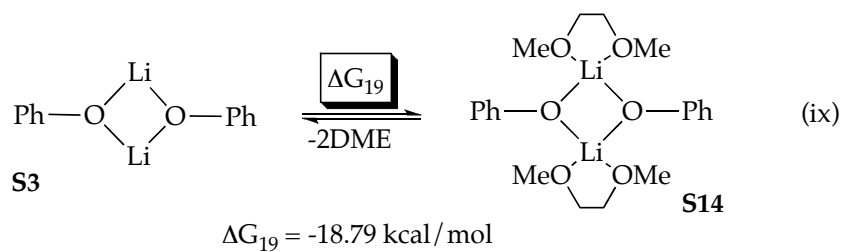


Dimer solvation

S=Me₂O

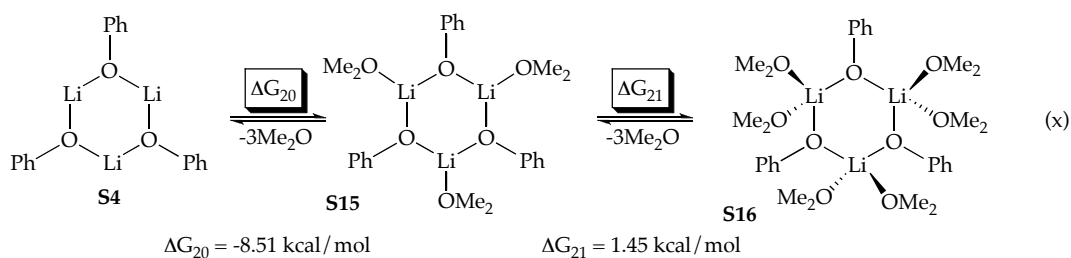


S=DME

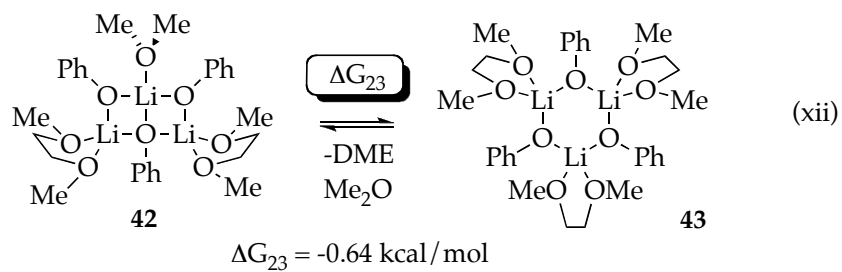
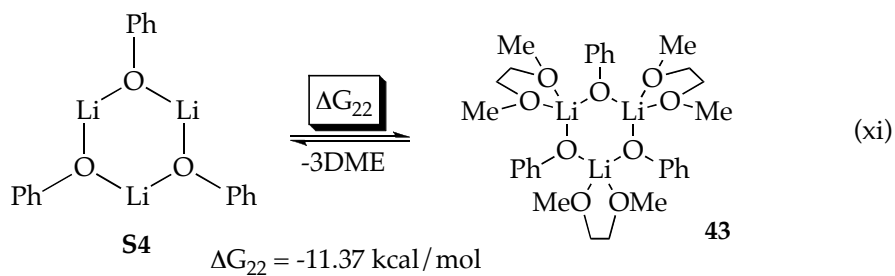


Trimer solvation

S=Me₂O

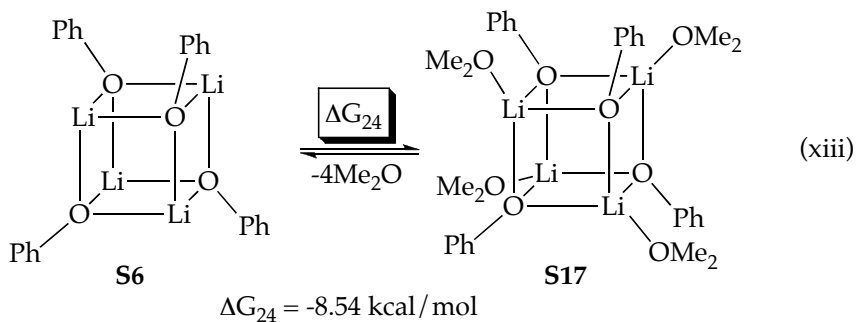


S=DME



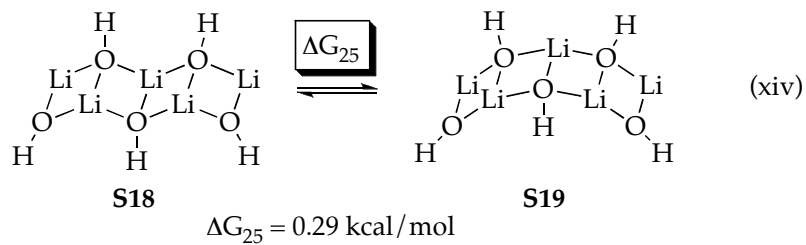
Tetramer solvation

$S=Me_2O$

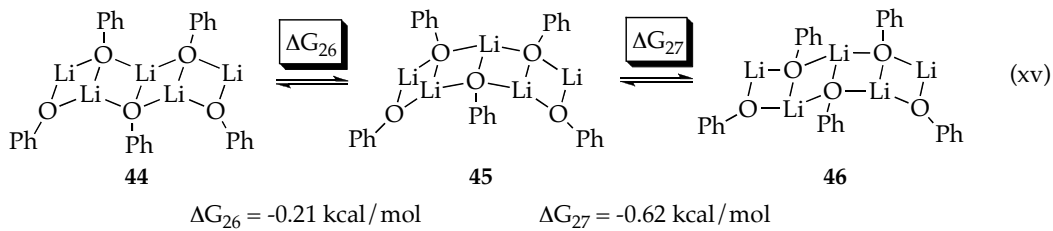


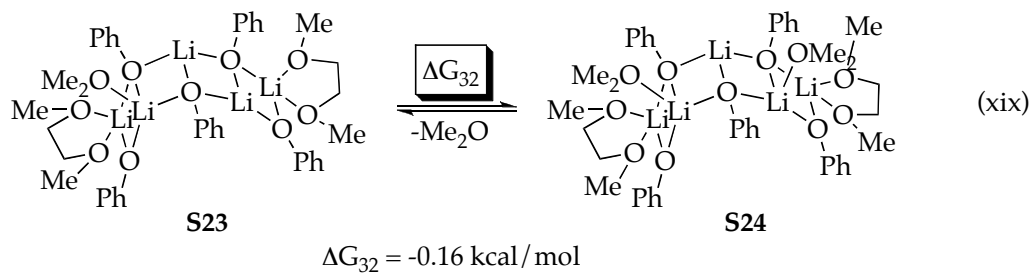
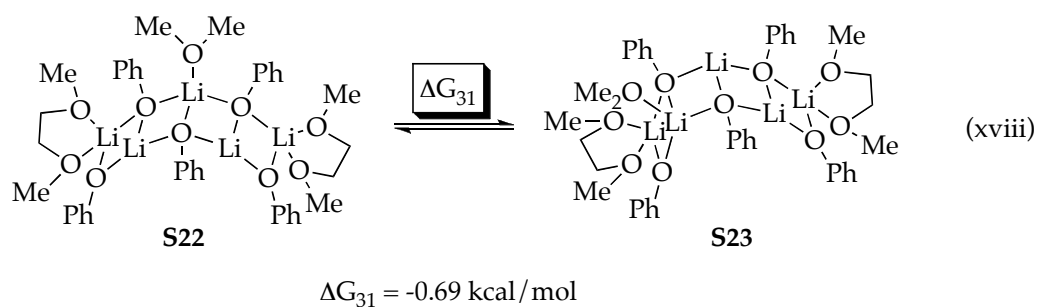
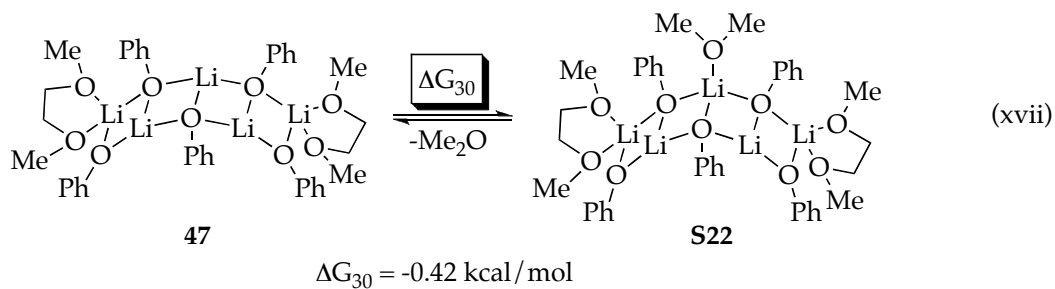
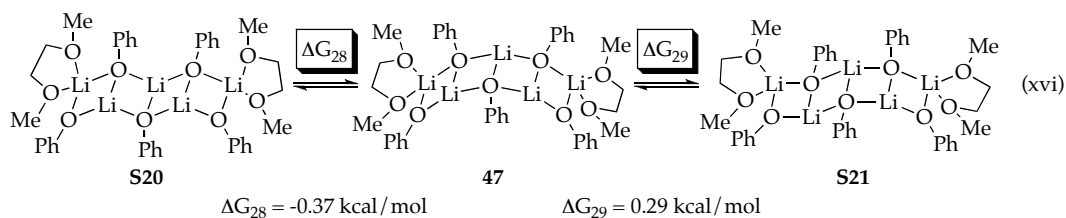
Determination of pentamer ladder shape and solvation

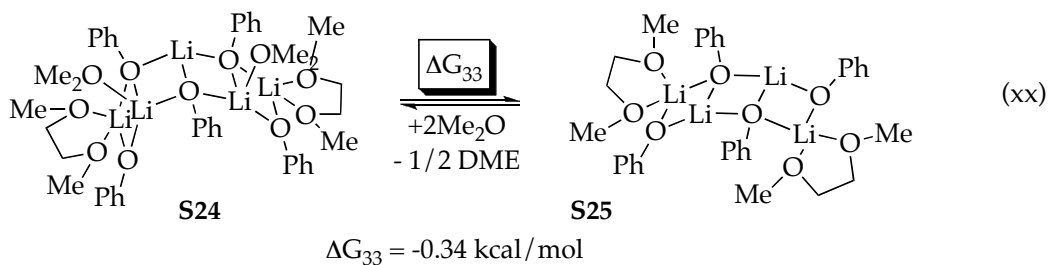
LiOH pentamers as a model system



PhOLi pentamers

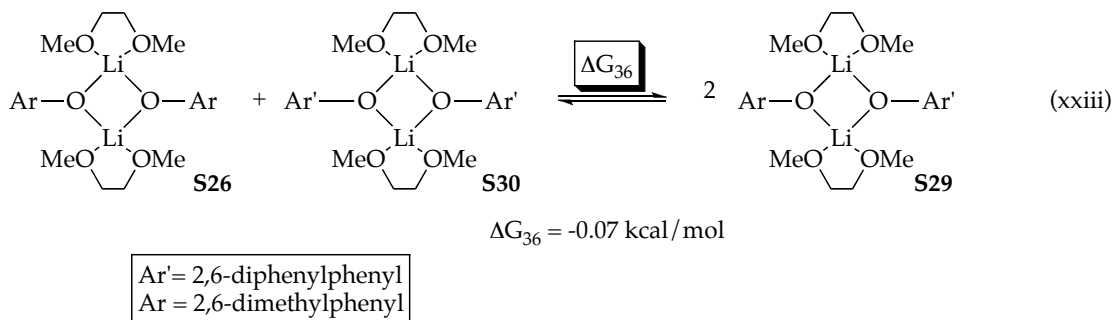
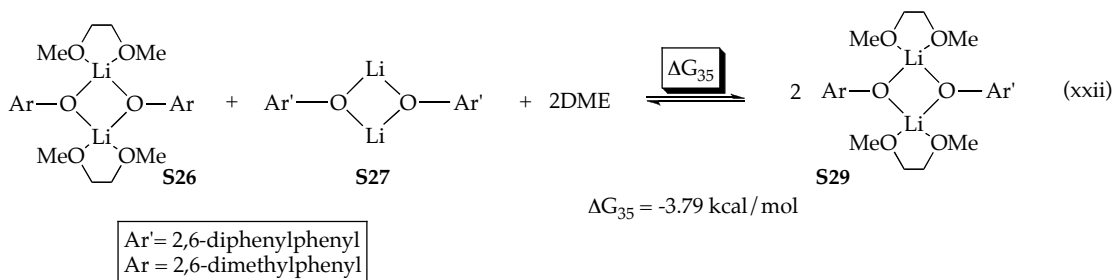
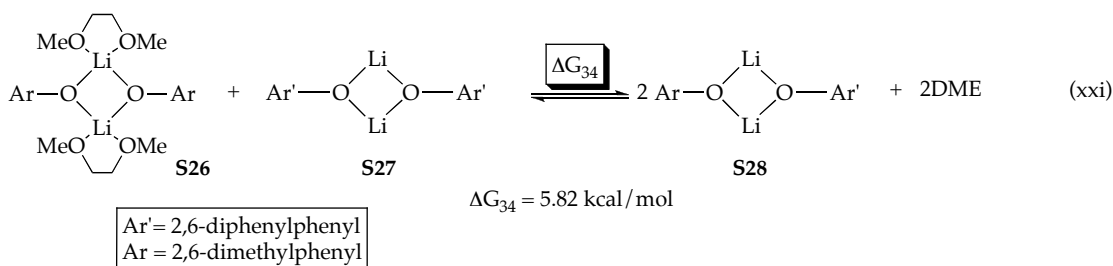


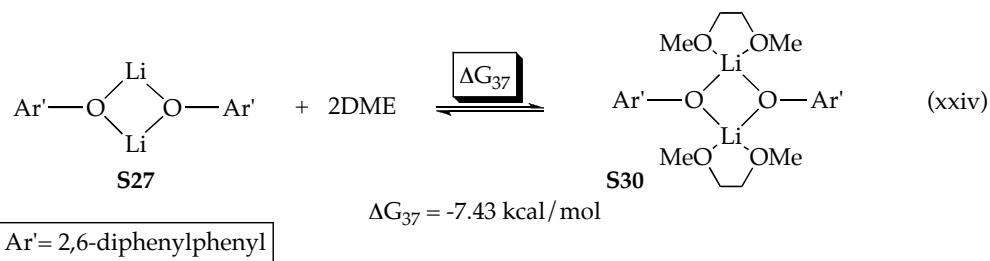




Others

Heterodimer formation from 2,6-dimethylphenolate and 2,6-diphenylphenolate





2,6-di-*tert*-butylphenolate solvation

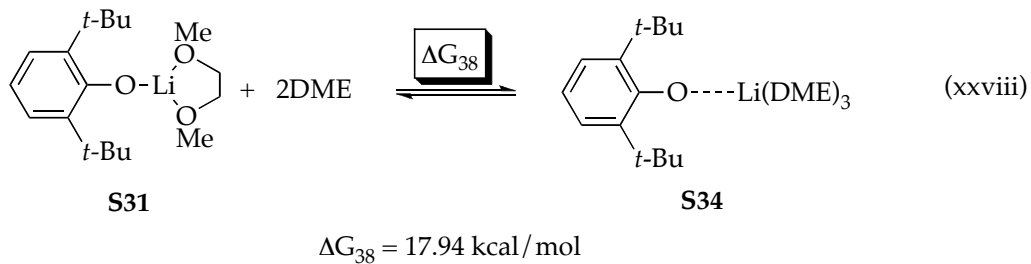
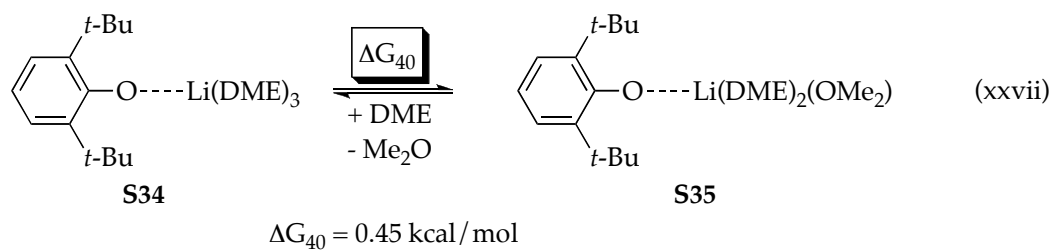
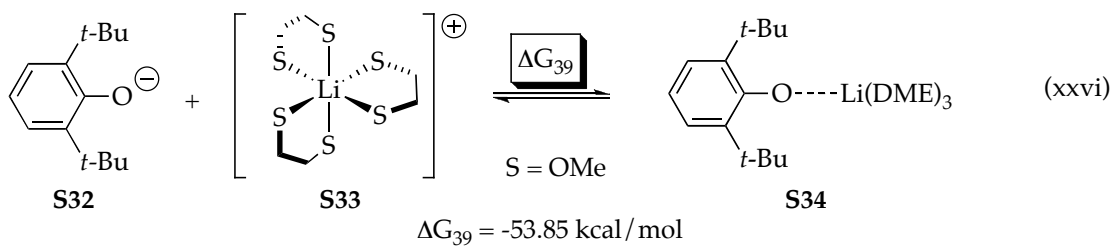
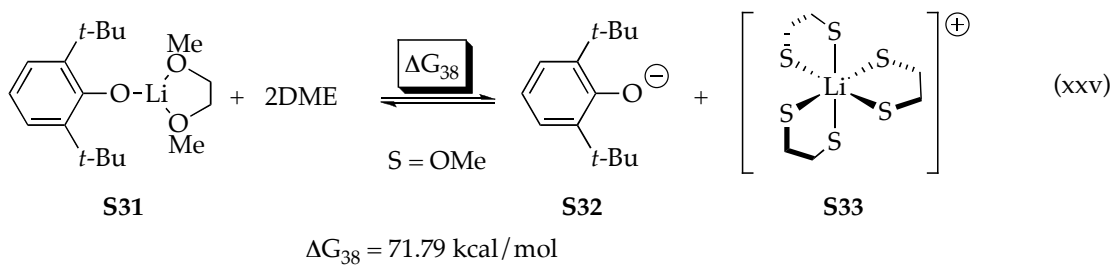
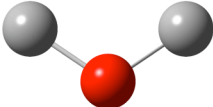
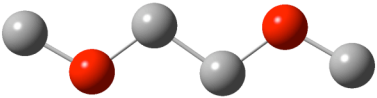


Table A1.5. Optimized geometry at B3LYP level of theory with 6-31G(d) basis set, free energy (G, Hartrees), and cartesian coordinates (X, Y, Z).

Me-O-Me		Me ₂ O G = -154.958697 (-90 °C)
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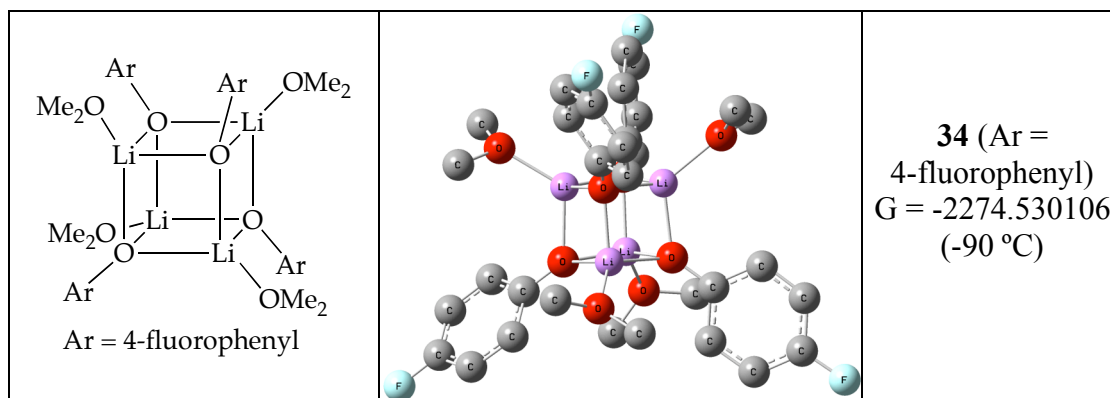
Atom	X	Y	Z
C	-1.170957	0.195262	0.000002
O	-0.000002	-0.589887	0.000011
C	1.170966	0.195268	-0.000001
H	1.232787	0.839156	0.893297
H	1.232018	0.840190	-0.892599
H	2.021804	-0.491398	-0.000758
H	-2.021793	-0.491404	-0.000504
H	-1.232665	0.839334	0.893177
H	-1.232188	0.840036	-0.892706

Table A1.5 (Continued).

<chem>COCCOC</chem>		DME $G = -308.730705$ (-90 °C)
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Atom	X	Y	Z
C	0.646680	-0.400765	-0.000050
O	1.719768	0.518926	-0.000258
C	2.980824	-0.113586	0.000175
H	3.121588	-0.744290	-0.892664
H	3.120984	-0.744247	0.893139
H	3.737943	0.675089	0.000414
C	-0.646681	0.400794	0.000034
O	-1.719758	-0.518928	-0.000176
C	-2.980825	0.113566	0.000130
H	-3.737931	-0.675122	-0.000006
H	-3.121203	0.744001	0.893220
H	-3.121393	0.744489	-0.892585
H	-0.679907	1.052031	-0.888944
H	-0.680064	1.051766	0.889196
H	0.679807	-1.051938	-0.889082
H	0.680113	-1.051816	0.889054

Table A1.5 (Continued).



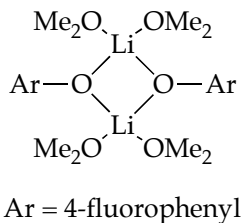
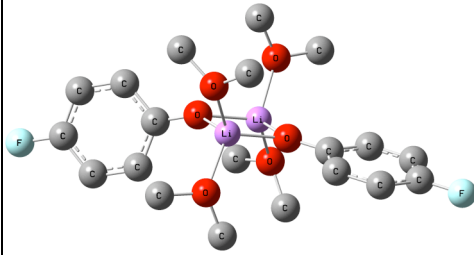
Atom	X	Y	Z	Atom	X	Y	Z
O	0.735744	0.150809	1.573617	H	3.361561	1.111041	-0.297515
Li	-0.017001	-1.448312	0.740469	H	4.344057	0.687785	-1.240599
O	-1.695349	-0.581158	0.196583	H	5.157250	0.150038	-0.735138
Li	-0.745702	-0.163833	-1.465126	C	3.849996	0.017080	-1.945639
O	-0.024207	1.540155	-0.840074	H	4.759334	1.552106	-1.776617
Li	-0.849327	1.053843	0.880420	H	3.887956	1.985545	0.698766
O	-1.796917	2.475885	1.877358	H	4.692678	1.493015	1.258957
C	-1.246558	3.792034	1.919375	C	4.271105	2.906038	0.237750
H	-1.459989	4.263700	2.887901	C	3.072861	2.224806	1.382987
H	-0.166947	3.695068	1.792759	C	-0.086855	2.720876	-1.452231
H	-1.651272	4.407918	1.107140	C	1.090128	3.423597	-1.797994
C	-3.209780	2.463345	2.076127	C	0.996948	4.653385	-2.432424
H	-3.535103	1.422875	2.026161	C	-0.215079	5.251637	-2.760649
H	-3.459625	2.880874	3.060853	H	-1.379983	4.556418	-2.424567
H	-3.717343	3.047192	1.296464	H	-1.329320	3.317515	-1.784561
Li	1.498159	0.474023	-0.207360	H	-2.245264	2.790086	-1.528694
O	0.846870	-1.204713	-0.996767	O	-2.346781	4.990880	-2.668129
C	1.614960	-2.001632	-1.737338	C	-0.233568	6.214964	-3.257430
C	2.162888	-3.189951	-1.201027	H	2.147226	5.299751	-2.746138
C	2.956013	-4.002237	-1.998333	H	2.061367	2.998906	-1.566874
C	3.258522	-3.708716	-3.323933	H	-1.571199	-0.448846	-3.240446
C	2.725881	-2.530169	-3.852921	C	-1.417477	0.467617	-4.322966
C	1.921701	-1.687243	-3.085250	H	-0.554558	0.194142	-4.945538
H	1.516442	-0.772134	-3.510415	H	-2.322157	0.476781	-4.945658
H	2.944229	-2.264714	-4.884759	H	-1.262383	1.457089	-3.889555
H	3.884163	-4.377859	-3.903772	C	-1.794704	-1.788371	-3.678772
O	3.459032	-5.137382	-1.454012	C	-1.962875	-2.394304	-2.786582
C	1.964006	-3.465274	-0.170206	C	-2.684255	-1.836052	-4.320844

C	-0.921824	-2.169839	-4.223165
C	-2.942473	-0.980349	0.438134
C	-3.915794	-0.990536	-0.587601
H	-5.205791	-1.416412	-0.307075

Table A1.5 (Continued).

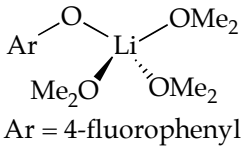
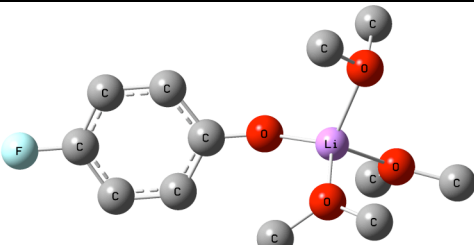
Atom	X	Y	Z
H	-5.612124	-1.838804	0.954341
H	-4.654677	-1.818908	1.972062
O	-3.346129	-1.399496	1.730835
C	-2.613468	-1.382574	2.534001
H	-4.937163	-2.135226	2.973508
H	-6.633425	-2.162217	1.120588
H	-6.112054	-1.418770	-1.315682
C	-3.655156	-0.659195	-1.587531
H	-0.087743	-3.230405	1.587431
H	-0.831078	-4.245944	0.914118
H	-1.887836	-4.213016	1.207939
C	-0.739019	-4.053244	-0.156392
C	-0.413555	-5.236193	1.139665
C	-0.063667	-3.411628	3.002536
C	0.388471	-4.380480	3.253585
C	0.544499	-2.607314	3.419761
C	-1.079476	-3.368106	3.417819
H	1.352599	0.184225	2.754704
H	0.861372	0.987474	3.808956
H	1.526453	1.004317	5.026471
F	2.673442	0.259171	5.278606
F	3.156961	-0.539318	4.238279
F	2.517961	-0.584212	2.999185
F	2.906605	-1.206955	2.197152
H	4.050545	-1.137933	4.398911
H	3.155619	0.308598	6.248352
H	1.029653	1.787067	6.015872
H	-0.037432	1.579090	3.668091

Table A1.5 (Continued).

 <p>Ar = 4-fluorophenyl</p>		<p>35 (Ar = 4-fluorophenyl) G = -1447.170703 (-90 °C)</p>
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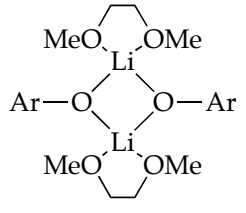
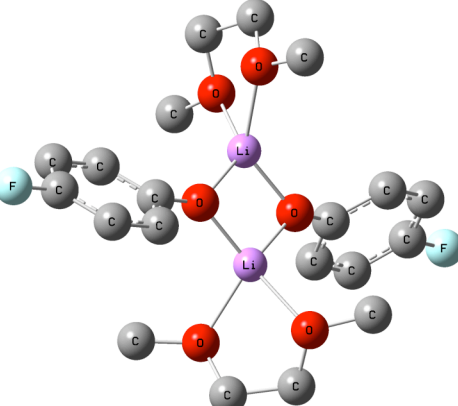
Atom	X	Y	Z	Atom	X	Y	Z
C	0.712005	2.348694	-2.488717	H	-2.058337	-3.016962	-1.788696
O	0.052675	2.673072	-1.268433	H	-1.393482	-3.806125	-0.327580
Li	0.080046	1.282401	0.199056	H	-0.911815	-4.389085	-1.947608
O	1.421497	-0.029965	0.050047	C	2.725180	-0.084700	-0.154282
Li	0.006549	-1.249657	0.220751	C	3.538030	1.077545	-0.107292
O	-1.353603	0.055344	0.364053	C	4.912328	1.014122	-0.329757
C	-2.626378	0.067943	0.003651	C	5.541185	-0.202736	-0.608522
C	-3.667535	0.202271	0.957272	C	4.759828	-1.360451	-0.661316
C	-5.007994	0.209199	0.573851	C	3.384528	-1.308647	-0.441680
C	-5.372992	0.084694	-0.769537	H	2.786054	-2.216461	-0.494713
C	-4.363633	-0.046098	-1.727643	H	5.227381	-2.319297	-0.878787
C	-3.019803	-0.054988	-1.355091	H	5.501093	1.928702	-0.282643
H	-2.238138	-0.154703	-2.105933	H	3.061761	2.030462	0.115601
H	-4.625560	-0.141738	-2.780087	C	-1.196404	3.330441	-1.472101
H	-6.418970	0.091086	-1.063174	H	-1.598612	3.560241	-0.483706
H	-3.393900	0.307998	2.005004	H	-1.052142	4.261788	-2.037571
O	-0.072037	-2.505366	1.810642	H	-1.900699	2.679027	-2.005217
C	1.121202	-2.981043	2.422053	H	0.926785	3.261255	-3.062503
H	0.987253	-4.008607	2.789198	H	1.646053	1.850213	-2.224534
H	1.905711	-2.958445	1.664219	H	0.093768	1.677842	-3.101827
H	1.414120	-2.334713	3.261281	O	0.066508	2.559243	1.772124
C	-1.161479	-2.412678	2.720594	C	-0.312044	1.952116	3.002671
H	-2.001669	-1.983043	2.173955	H	-1.000288	1.146099	2.744934
H	-1.429130	-3.406676	3.106869	H	-0.809377	2.681847	3.657407
H	-0.908223	-1.758090	3.566967	H	0.566005	1.541427	3.521714
O	-0.077860	-2.598371	-1.289081	C	1.022167	3.597698	1.935839
C	0.354783	-2.162190	-2.573127	H	1.234758	3.992728	0.940736
H	-0.461989	-1.663872	-3.114447	H	0.619767	4.399727	2.571109
H	0.711332	-3.014334	-3.168872	H	1.948883	3.213478	2.384846
H	1.172849	-1.459897	-2.408000	F	6.902589	-0.259595	-0.827029
C	-1.175158	-3.502813	-1.353063	F	-5.984603	0.343907	1.539504

Table A1.5 (Continued).

 <p>Ar = 4-fluorophenyl</p>		<p>36 (Ar = 4-fluorophenyl) G = -878.527894 (-90 °C)</p>
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Atom	X	Y	Z	Atom	X	Y	Z
Li	1.407914	0.042926	-0.016230	O	2.302122	1.863833	0.116697
O	-0.249428	0.079559	-0.608913	C	2.267815	2.484653	-1.169042
O	2.533308	-0.935191	-1.381516	H	2.773431	3.459627	-1.137977
C	1.762198	-1.561106	-2.410325	H	2.793730	1.818771	-1.855218
H	1.811664	-2.655079	-2.315380	H	1.231661	2.610806	-1.507309
H	0.738442	-1.212769	-2.263741	C	1.638998	2.652073	1.104793
H	2.138585	-1.268780	-3.400711	H	0.583969	2.798289	0.839885
C	3.898778	-1.311292	-1.397052	H	1.702105	2.101582	2.044966
H	4.014701	-2.392298	-1.231167	H	2.132672	3.627681	1.213011
H	4.369254	-1.049548	-2.355972	C	-1.550318	0.035861	-0.440959
H	4.397890	-0.765474	-0.592624	C	-2.252288	-1.197599	-0.348051
O	1.641266	-0.701826	1.839799	C	-3.634212	-1.250215	-0.165355
C	2.841078	-0.936062	2.558412	C	-4.354370	-0.066095	-0.074789
H	2.741629	-0.614293	3.605028	C	-3.719819	1.167357	-0.166199
H	3.112716	-2.001528	2.540812	C	-2.338926	1.215124	-0.348186
H	3.627901	-0.350763	2.076575	H	-1.835501	2.175666	-0.434209
C	0.515027	-1.386797	2.390399	H	-4.311045	2.076612	-0.097031
H	0.322850	-1.042769	3.416046	F	-5.705248	-0.113668	0.105843
H	-0.338340	-1.157601	1.751708	H	-4.158242	-2.199876	-0.096926
H	0.691540	-2.471563	2.402319	H	-1.680022	-2.118875	-0.436393

Table A1.5 (Continued).

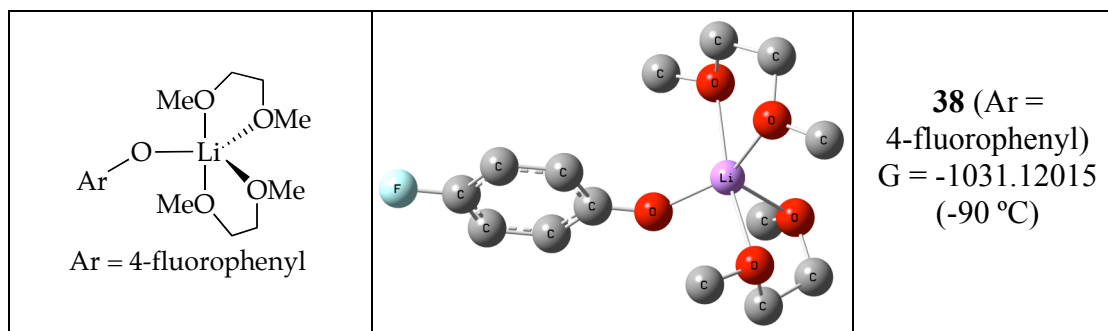
 <p>Ar = 4-fluorophenyl</p>		<p>37 (Ar = 4-fluorophenyl) G = -1444.809759 (-90 °C)</p>
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Atom	X	Y	Z	Atom	X	Y	Z
Li	0.006243	-1.242034	0.194769	H	-5.388604	1.226842	-1.694250
O	-0.262288	-2.783350	-1.143046	H	-2.890605	1.342308	-1.580848
C	-0.129667	-4.032806	-0.476716	Li	-0.047593	1.281600	0.159552
C	0.958394	-3.876735	0.565856	O	1.347151	0.055556	0.281737
O	0.559213	-2.824066	1.437518	C	2.653889	0.063483	0.074390
C	1.527798	-2.529811	2.444334	C	3.231027	-0.577159	-1.052134
H	1.691905	-3.407399	3.084648	C	4.609246	-0.577073	-1.270129
H	2.475831	-2.211072	1.994986	C	5.441203	0.065586	-0.361813
H	1.121019	-1.712136	3.040748	C	4.924282	0.706302	0.757724
H	1.081136	-4.817086	1.124034	C	3.545909	0.702397	0.972122
H	1.916455	-3.623484	0.087685	H	3.128871	1.193607	1.848233
H	-1.081155	-4.303172	0.005572	H	5.601239	1.198997	1.450035
H	0.139627	-4.827141	-1.189106	F	6.786120	0.067497	-0.571768
C	-1.369904	-2.730126	-2.040891	H	5.043215	-1.067569	-2.137039
H	-2.310890	-2.922542	-1.510224	H	2.567029	-1.069735	-1.759373
H	-1.243334	-3.460461	-2.851697	O	0.427216	2.817139	-1.127871
H	-1.394061	-1.719623	-2.449207	C	-0.286189	3.988018	-0.754605
O	-1.386718	-0.017096	0.095462	C	-0.175008	4.111929	0.753115
C	-2.707322	-0.069493	0.039121	O	-0.637810	2.888982	1.309303
C	-3.442153	0.698609	-0.898713	C	-0.636040	2.860444	2.731002
C	-4.833711	0.636182	-0.970658	H	-1.298141	3.637954	3.135663
C	-5.522171	-0.201612	-0.102014	H	-1.009969	1.877803	3.022934
C	-4.848128	-0.974539	0.835511	H	0.378739	3.004807	3.127919
C	-3.456459	-0.906630	0.904173	H	-0.786997	4.955372	1.106268
H	-2.918577	-1.496391	1.643382	H	0.870984	4.288337	1.046632
H	-5.414625	-1.617105	1.503745	H	-1.340758	3.901200	-1.057672
F	-6.880171	-0.266530	-0.171263	H	0.146567	4.877840	-1.235666

Table A1.5 (Continued).

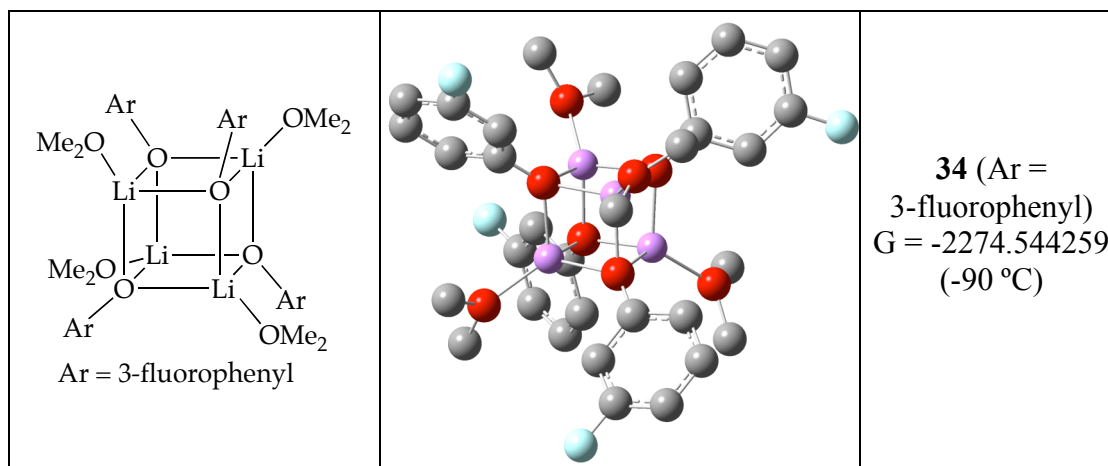
Atom	X	Y	Z
C	0.501494	2.598224	-2.531819
H	-0.500551	2.474648	-2.966333
H	1.081158	1.684394	-2.671067
H	1.011951	3.434960	-3.027632

Table A1.5 (Continued).



Atom	X	Y	Z	Atom	X	Y	Z
Li	-1.198501	0.067794	0.084324	H	-1.209352	3.997120	0.635242
O	0.455603	-0.624172	0.319410	H	-0.308935	3.010566	-0.548526
C	1.734756	-0.431380	0.112938	C	0.291949	2.165627	1.852071
C	2.219249	0.428490	-0.914044	H	0.386488	1.321312	2.534043
C	3.582796	0.633137	-1.129084	H	0.274701	3.107162	2.419558
C	4.504565	-0.018723	-0.320497	H	1.144035	2.156226	1.163043
C	4.088302	-0.870821	0.696547	O	-2.483202	-0.985956	1.408452
C	2.726207	-1.072183	0.908242	C	-2.878444	-2.209535	0.780161
H	2.391228	-1.739056	1.699588	C	-1.866414	-2.678970	-0.250782
H	4.833580	-1.367372	1.312340	O	-1.822085	-1.688474	-1.273523
F	5.838314	0.179306	-0.526793	C	-0.817722	-1.960586	-2.250832
H	3.936693	1.290548	-1.918997	H	0.174007	-1.945848	-1.788561
H	1.490412	0.928533	-1.550077	H	-1.003803	-2.930143	-2.735336
O	-0.937575	1.994899	1.144292	H	-0.883118	-1.167830	-2.999909
C	-1.144848	3.001510	0.167939	H	-0.869000	-2.785690	0.194723
C	-2.443275	2.690607	-0.543981	H	-2.184054	-3.648527	-0.668839
O	-2.332832	1.389281	-1.109546	H	-3.041543	-2.989055	1.536933
C	-3.504012	0.992597	-1.815895	H	-3.833816	-2.004628	0.285425
H	-3.341317	-0.035420	-2.137581	C	-1.721512	-1.165612	2.608943
H	-4.387219	1.037549	-1.162515	H	-0.725050	-1.560459	2.385897
H	-3.669365	1.643080	-2.686142	H	-2.259539	-1.824094	3.304157
H	-3.284311	2.717252	0.165306	H	-1.621889	-0.175062	3.056879
H	-2.627003	3.437142	-1.331547				

Table A1.5 (Continued).

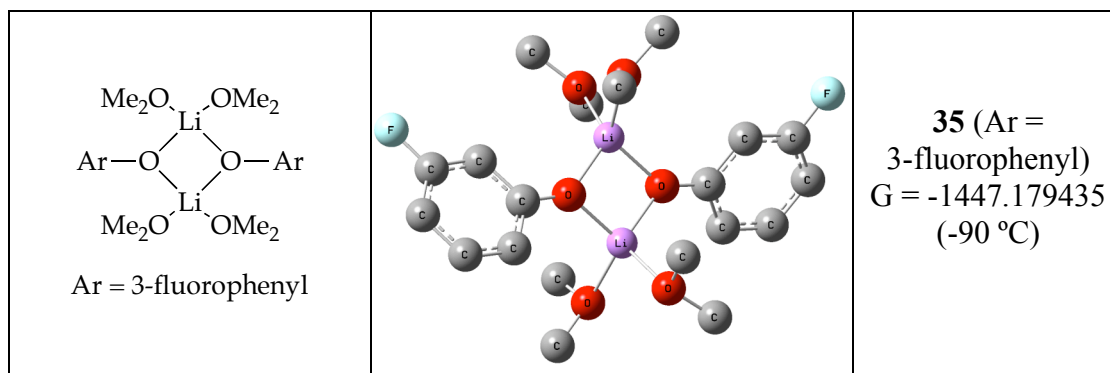


Atom	X	Y	Z	Atom	X	Y	Z
O	0.735744	0.150809	1.573617	H	1.964006	-3.465274	-0.170206
Li	-0.017001	-1.448312	0.740469	O	3.361561	1.111041	-0.297515
O	-1.695349	-0.581158	0.196583	C	4.344057	0.687785	-1.240599
Li	-0.745702	-0.163833	-1.465126	H	5.157250	0.150038	-0.735138
O	-0.024207	1.540155	-0.840074	H	3.849996	0.017080	-1.945639
Li	-0.849327	1.053843	0.880420	H	4.759334	1.552106	-1.776617
O	-1.796917	2.475885	1.877358	C	3.887956	1.985545	0.698766
C	-1.246558	3.792034	1.919375	H	4.692678	1.493015	1.258957
H	-1.459989	4.263700	2.887901	H	4.271105	2.906038	0.237750
H	-0.166947	3.695068	1.792759	H	3.072861	2.224806	1.382987
H	-1.651272	4.407918	1.107140	C	-0.086855	2.720876	-1.452231
C	-3.209780	2.463345	2.076127	C	1.090128	3.423597	-1.797994
H	-3.535103	1.422875	2.026161	C	0.996948	4.653385	-2.432424
H	-3.459625	2.880874	3.060853	C	-0.215079	5.251637	-2.760649
H	-3.717343	3.047192	1.296464	C	-1.379983	4.556418	-2.424567
Li	1.498159	0.474023	-0.207360	C	-1.329320	3.317515	-1.784561
O	0.846870	-1.204713	-0.996767	H	-2.245264	2.790086	-1.528694
C	1.614960	-2.001632	-1.737338	H	-2.346781	4.990880	-2.668129
C	2.162888	-3.189951	-1.201027	H	-0.233568	6.214964	-3.257430
C	2.956013	-4.002237	-1.998333	F	2.147226	5.299751	-2.746138
C	3.258522	-3.708716	-3.323933	H	2.061367	2.998906	-1.566874
C	2.725881	-2.530169	-3.852921	O	-1.571199	-0.448846	-3.240446
C	1.921701	-1.687243	-3.085250	C	-1.417477	0.467617	-4.322966
H	1.516442	-0.772134	-3.510415	H	-0.554558	0.194142	-4.945538
H	2.944229	-2.264714	-4.884759	H	-2.322157	0.476781	-4.945658
H	3.884163	-4.377859	-3.903772	H	-1.262383	1.457089	-3.889555
F	3.459032	-5.137382	-1.454012	C	-1.794704	-1.788371	-3.678772

Table A1.5 (Continued).

Atom	X	Y	Z
H	-1.962875	-2.394304	-2.786582
H	-2.684255	-1.836052	-4.320844
H	-0.921824	-2.169839	-4.223165
C	-2.942473	-0.980349	0.438134
C	-3.915794	-0.990536	-0.587601
C	-5.205791	-1.416412	-0.307075
C	-5.612124	-1.838804	0.954341
C	-4.654677	-1.818908	1.972062
C	-3.346129	-1.399496	1.730835
H	-2.613468	-1.382574	2.534001
H	-4.937163	-2.135226	2.973508
H	-6.633425	-2.162217	1.120588
F	-6.112054	-1.418770	-1.315682
H	-3.655156	-0.659195	-1.587531
O	-0.087743	-3.230405	1.587431
C	-0.831078	-4.245944	0.914118
H	-1.887836	-4.213016	1.207939
H	-0.739019	-4.053244	-0.156392
H	-0.413555	-5.236193	1.139665
C	-0.063667	-3.411628	3.002536
H	0.388471	-4.380480	3.253585
H	0.544499	-2.607314	3.419761
H	-1.079476	-3.368106	3.417819
C	1.352599	0.184225	2.754704
C	0.861372	0.987474	3.808956
C	1.526453	1.004317	5.026471
C	2.673442	0.259171	5.278606
C	3.156961	-0.539318	4.238279
C	2.517961	-0.584212	2.999185
H	2.906605	-1.206955	2.197152
H	4.050545	-1.137933	4.398911
H	3.155619	0.308598	6.248352
F	1.029653	1.787067	6.015872
H	-0.037432	1.579090	3.668091

Table A1.5 (Continued).

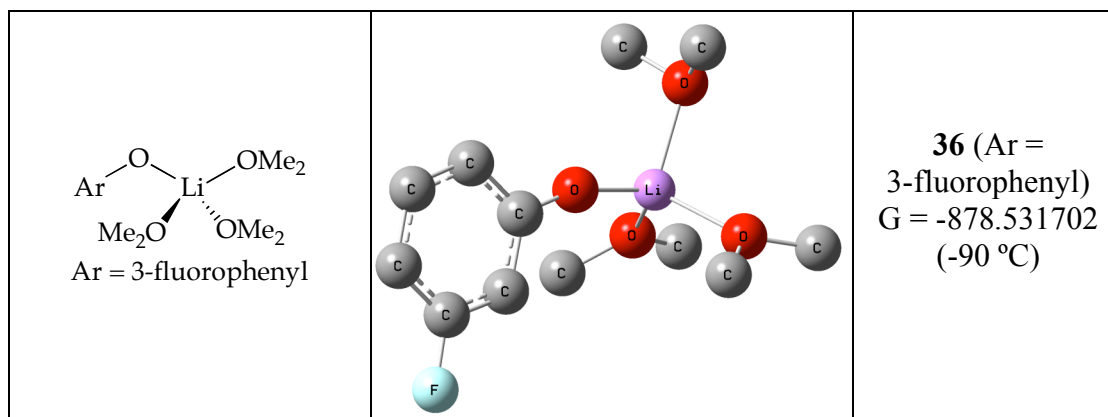


Atom	X	Y	Z	Atom	X	Y	Z
C	1.458824	3.479209	-1.593307	H	-1.506113	-3.024243	2.605583
O	0.275448	2.683630	-1.585101	H	-1.317371	-3.659031	0.943165
Li	0.018402	1.432308	-0.015548	C	0.983440	-2.076774	2.680157
O	1.378282	0.139699	0.128705	H	1.512603	-2.945249	3.096248
Li	-0.007119	-1.140366	0.018519	H	1.702993	-1.336906	2.329574
O	-1.369584	0.164424	-0.137338	H	0.346662	-1.637732	3.461692
C	-2.685451	0.225129	-0.184624	C	2.694339	0.188485	0.199758
C	-3.363993	1.359074	-0.708871	C	3.505283	-0.802802	-0.409044
C	-4.754724	1.410387	-0.758984	C	4.886199	-0.728823	-0.309270
C	-5.543171	0.350814	-0.299028	C	5.549033	0.288046	0.369170
C	-4.873838	-0.756345	0.210536	C	4.755553	1.269960	0.970856
C	-3.491920	-0.845797	0.278417	C	3.365588	1.230634	0.895105
H	-3.030350	-1.734966	0.695851	H	2.764850	2.000893	1.372907
F	-5.606304	-1.805211	0.667494	H	5.236804	2.081209	1.512874
H	-6.626735	0.371065	-0.330508	H	6.632100	0.299797	0.418405
H	-5.240694	2.293320	-1.168611	F	5.624598	-1.699406	-0.908037
H	-2.769176	2.191134	-1.078144	H	3.047968	-1.617542	-0.961267
O	-0.239844	-2.538759	-1.440260	O	-0.222471	2.740206	1.515323
C	0.775119	-3.489968	-1.734282	C	-1.255588	3.715881	1.401007
H	1.463518	-3.108196	-2.501513	H	-1.154856	4.476748	2.187488
H	0.333879	-4.432799	-2.087380	H	-2.246055	3.247033	1.466041
H	1.323745	-3.667904	-0.807686	H	-1.141793	4.185120	0.421909
C	-1.045568	-2.220671	-2.571334	C	-0.255950	2.056757	2.765832
H	-0.433532	-1.787871	-3.375609	H	-0.104396	2.762739	3.594213
H	-1.786391	-1.494049	-2.237766	H	-1.213265	1.535253	2.898902
H	-1.549670	-3.120696	-2.949802	H	0.557498	1.329697	2.747408
O	0.203644	-2.461201	1.551629	C	0.064862	2.006984	-2.822387
C	-0.792796	-3.423563	1.870880	H	0.920812	1.361825	-3.062986
H	-0.335482	-4.337537	2.275692	H	-0.086335	2.730503	-3.635526

Table A1.5 (Continued).

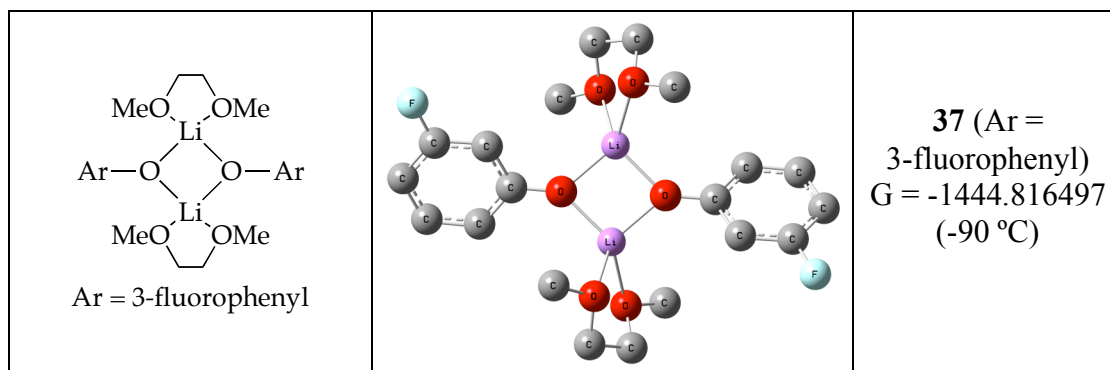
Atom	X	Y	Z
H	-0.830192	1.395632	-2.697504
H	2.349751	2.856143	-1.743525
H	1.403661	4.241711	-2.382722
H	1.521829	3.966928	-0.618629

Table A1.5 (Continued).



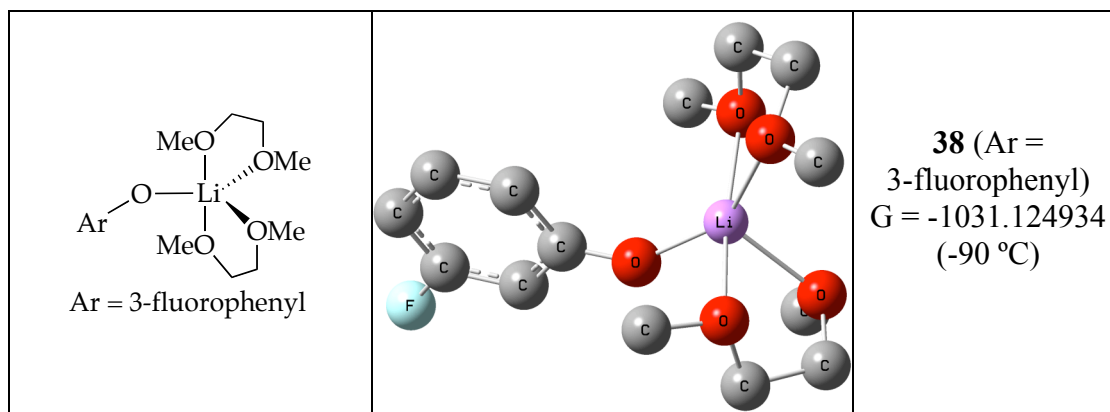
Atom	X	Y	Z	Atom	X	Y	Z
Li	1.378461	0.048354	0.000246	C	2.337501	2.415802	-1.180218
O	1.857924	-0.968527	-1.669990	H	2.973556	3.311018	-1.212283
C	0.747467	-1.326298	-2.495390	H	2.572237	1.768830	-2.027394
H	0.595219	-2.414478	-2.486363	H	1.279688	2.703153	-1.222708
H	-0.122490	-0.822346	-2.074063	C	2.328488	2.417987	1.183919
H	0.917641	-0.995186	-3.529305	H	1.270285	2.705057	1.217996
C	3.074961	-1.567570	-2.081782	H	2.557170	1.772771	2.034087
H	3.014166	-2.664308	-2.031321	H	2.963958	3.313503	1.218950
H	3.329379	-1.274928	-3.110710	O	-0.300665	0.582950	-0.009208
H	3.857884	-1.215467	-1.405699	C	-1.607031	0.553549	-0.006606
O	1.843502	-0.964730	1.676854	C	-2.326991	-0.674171	-0.005614
C	3.056991	-1.564801	2.097604	C	-3.713256	-0.670558	-0.002791
H	3.303569	-1.273100	3.128702	C	-4.474469	0.492256	-0.000819
H	2.995960	-2.661461	2.045787	C	-3.774351	1.705412	-0.001864
H	3.845291	-1.212580	1.427867	C	-2.384769	1.746460	-0.004676
C	0.726474	-1.322962	2.493098	H	-1.857533	2.697345	-0.005611
H	0.888176	-0.992172	3.528469	H	-4.335095	2.638129	-0.000450
H	-0.140407	-0.819343	2.065142	H	-5.557594	0.440893	0.001356
H	0.574498	-2.411165	2.482505	F	-4.358074	-1.869871	-0.001921
O	2.600043	1.660066	0.003572	H	-1.790781	-1.619100	-0.007394

Table A1.5 (Continued).



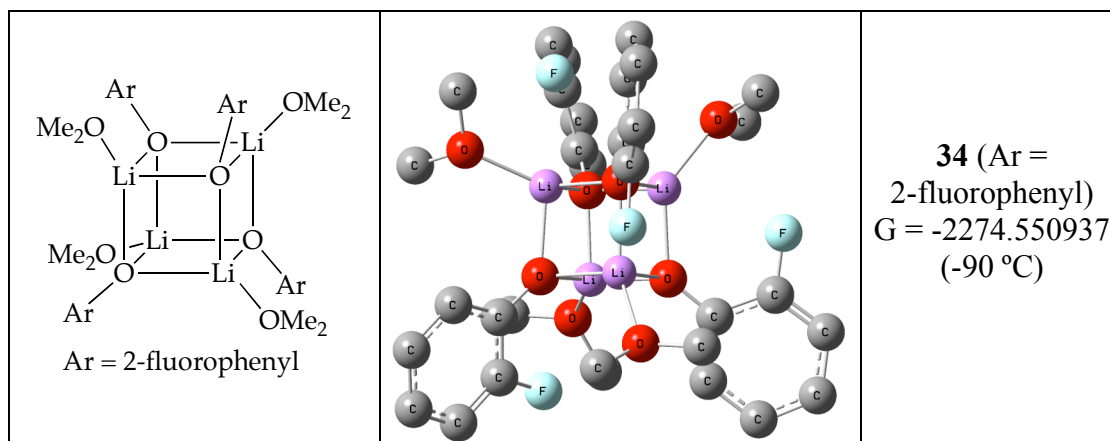
Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.280725	-1.237855	0.125577	H	-0.671041	3.720187	-2.816497
O	1.335896	-0.307888	0.120693	H	-0.921005	1.963608	-2.576444
Li	0.280725	1.237855	0.125577	C	2.629805	-0.551570	0.100413
O	-1.335896	0.307888	0.120692	C	3.199188	-1.628822	0.830740
C	-2.629805	0.551570	0.100412	C	4.570191	-1.872302	0.803867
C	-3.199188	1.628821	0.830739	C	5.442157	-1.068001	0.062507
C	-4.570191	1.872301	0.803867	C	4.877685	-0.015208	-0.649450
C	-5.442157	1.068000	0.062507	C	3.518065	0.259116	-0.652460
C	-4.877685	0.015208	-0.649450	H	3.130954	1.080647	-1.248395
C	-3.518065	-0.259116	-0.652461	F	5.695127	0.786818	-1.380452
H	-3.130953	-1.080647	-1.248395	H	6.512311	-1.239611	0.031501
F	-5.695127	-0.786819	-1.380451	H	4.975303	-2.703115	1.377601
H	-6.512311	1.239610	0.031501	H	2.536891	-2.250450	1.428987
H	-4.975304	2.703114	1.377601	O	-0.233726	-2.844113	-1.156595
H	-2.536892	2.250450	1.428987	C	0.855622	-2.930288	-2.075947
O	0.233727	2.844114	-1.156595	H	0.921005	-1.963608	-2.576444
C	0.434764	4.034436	-0.403269	H	1.796623	-3.125223	-1.546658
C	1.514084	3.746513	0.620650	H	0.671040	-3.720187	-2.816497
O	1.066961	2.649322	1.409553	C	-0.434764	-4.034436	-0.403269
C	2.023857	2.223033	2.380193	C	-1.514084	-3.746512	0.620650
H	2.223687	3.028711	3.099661	O	-1.066961	-2.649322	1.409553
H	1.586081	1.368208	2.896995	C	-2.023857	-2.223033	2.380193
H	2.958085	1.912896	1.896689	H	-2.223687	-3.028711	3.099662
H	2.459564	3.487806	0.121133	H	-1.586081	-1.368208	2.896996
H	1.681161	4.634082	1.249276	H	-2.958085	-1.912896	1.896690
H	0.747428	4.860793	-1.059113	H	-1.681161	-4.634082	1.249276
H	-0.500780	4.321941	0.099943	H	-2.459564	-3.487805	0.121133
C	-0.855622	2.930289	-2.075947	H	0.500780	-4.321940	0.099943
H	-1.796623	3.125223	-1.546658	H	-0.747428	-4.860792	-1.059113

Table A1.5 (Continued).



Atom	X	Y	Z	Atom	X	Y	Z
Li	-1.153085	0.036651	0.091490	H	-1.532697	3.908961	0.833618
O	0.576143	-0.506063	0.121610	H	-0.690690	3.102813	-0.517410
C	1.797434	-0.175294	-0.198233	C	0.334076	2.234747	1.728724
C	2.088636	0.716139	-1.274338	H	0.626375	1.376777	2.332914
C	3.397157	1.060896	-1.601562	H	0.277104	3.136213	2.355378
C	4.488412	0.551196	-0.890186	H	1.078094	2.373688	0.936017
C	4.202295	-0.318283	0.158577	O	-2.163441	-1.174346	1.512829
C	2.916758	-0.686821	0.517204	C	-2.512020	-2.415802	0.892150
H	2.761070	-1.372676	1.344532	C	-1.586545	-2.759839	-0.262202
F	5.241217	-0.831698	0.872375	O	-1.750861	-1.742649	-1.245759
H	5.515031	0.805652	-1.129026	C	-0.848785	-1.892604	-2.341684
H	3.577586	1.741600	-2.431598	H	0.185869	-1.801576	-1.997142
H	1.253452	1.115551	-1.847194	H	-1.005485	-2.860045	-2.840560
O	-0.950202	1.937894	1.176197	H	-1.070685	-1.086629	-3.045284
C	-1.412323	2.952455	0.300395	H	-0.539055	-2.784599	0.064612
C	-2.749649	2.509681	-0.252277	H	-1.860949	-3.743563	-0.677743
O	-2.564833	1.254810	-0.897824	H	-2.511270	-3.224949	1.635055
C	-3.765252	0.746267	-1.470942	H	-3.533312	-2.294062	0.515687
H	-3.530339	-0.244312	-1.858434	C	-1.262969	-1.307223	2.619587
H	-4.555962	0.664902	-0.711273	H	-0.266716	-1.610496	2.281981
H	-4.114139	1.401050	-2.281672	H	-1.664446	-2.021599	3.350863
H	-3.484150	2.403984	0.560415	H	-1.198943	-0.319366	3.079664
H	-3.125241	3.257750	-0.966958				

Table A1.5 (Continued).

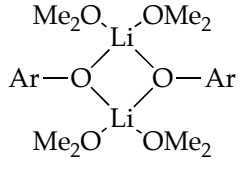
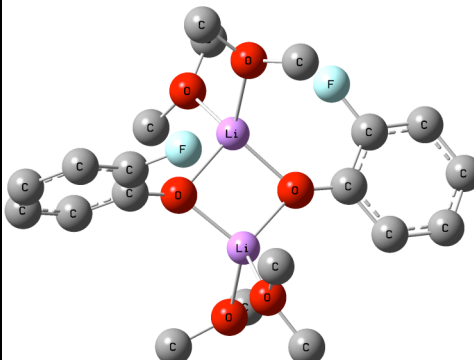


Atom	X	Y	Z	Atom	X	Y	Z
Li	-1.131471	0.810447	0.787185	H	0.610647	1.606726	-3.681242
O	-0.987765	0.833110	-1.198929	C	2.282027	-1.529222	-1.513018
Li	-0.725424	-1.124095	-1.052409	C	3.538563	-0.885000	-1.550878
O	-0.926484	-1.170829	0.890505	C	4.684275	-1.448624	-2.082098
Li	1.010576	-0.820464	1.017547	C	4.620465	-2.740446	-2.617861
O	1.223863	-0.930785	-0.984264	C	3.402842	-3.422345	-2.598105
Li	0.956615	1.010868	-0.918915	C	2.257087	-2.833211	-2.056103
O	0.813719	1.132889	1.034904	H	1.309697	-3.364560	-2.038656
C	1.417690	2.084002	1.735792	H	3.339672	-4.427754	-3.007907
C	0.672928	3.082333	2.398648	H	5.510010	-3.199182	-3.038880
C	1.233991	4.101477	3.146257	H	5.609930	-0.880145	-2.066860
C	2.627115	4.171161	3.261739	F	3.604932	0.380233	-1.023305
C	3.409890	3.213859	2.614606	O	2.581824	-1.660187	1.941533
C	2.821375	2.190986	1.864231	C	2.809167	-3.053870	1.745920
H	3.433669	1.455932	1.348344	H	3.864140	-3.297882	1.930920
H	4.493738	3.259446	2.690132	H	2.171161	-3.645718	2.414771
H	3.085314	4.963845	3.845357	H	2.570098	-3.276537	0.704781
H	0.582587	4.827351	3.624579	C	2.944336	-1.231093	3.252057
F	-0.690835	3.019669	2.275358	H	2.741623	-0.160389	3.308627
O	1.660988	2.425912	-2.146927	H	2.358634	-1.761916	4.012842
C	2.780292	3.252204	-1.837037	H	4.014938	-1.407095	3.425697
H	2.656915	4.244434	-2.292757	C	-1.715988	-1.962580	1.604312
H	2.819152	3.348178	-0.750903	C	-1.261080	-2.570579	2.793856
H	3.711977	2.797240	-2.196057	C	-2.034357	-3.404275	3.583047
C	1.518987	2.195795	-3.544143	C	-3.352818	-3.672684	3.199880
H	1.414353	3.147508	-4.083135	C	-3.852911	-3.086969	2.034921
H	2.385189	1.648084	-3.940764	C	-3.055183	-2.247754	1.253238

Table A1.5 (Continued).

Atom	X	Y	Z
H	-3.453744	-1.773859	0.360098
H	-4.878844	-3.279196	1.729928
H	-3.973609	-4.324620	3.806974
H	-1.601349	-3.830612	4.483524
F	0.028276	-2.305193	3.174766
O	-1.162336	-2.610286	-2.352056
C	-0.984793	-2.273901	-3.723639
H	-1.883392	-1.786892	-4.125140
H	-0.136009	-1.589422	-3.777004
H	-0.760234	-3.171867	-4.315607
C	-2.208444	-3.555757	-2.150400
H	-2.292096	-3.720111	-1.074910
H	-3.162027	-3.171932	-2.535361
H	-1.968145	-4.503569	-2.652167
C	-1.927715	1.454663	-1.895619
C	-3.102589	0.779862	-2.295739
C	-4.130987	1.366539	-3.010816
C	-4.024454	2.715236	-3.369568
C	-2.883897	3.428341	-2.994917
C	-1.856837	2.814913	-2.272661
H	-0.972657	3.373214	-1.976902
H	-2.789819	4.477681	-3.264119
H	-4.822104	3.193837	-3.929485
H	-5.001268	0.771279	-3.272507
F	-3.210183	-0.543219	-1.942512
O	-2.906600	1.329076	1.600902
C	-3.093923	1.041150	2.984191
H	-4.158949	0.881842	3.200318
H	-2.546743	0.123059	3.202207
H	-2.711271	1.861682	3.605119
C	-3.615507	2.497115	1.195789
H	-3.270015	3.375232	1.756973
H	-3.422822	2.641827	0.132230
H	-4.693909	2.362030	1.357312

Table A1.5 (Continued).

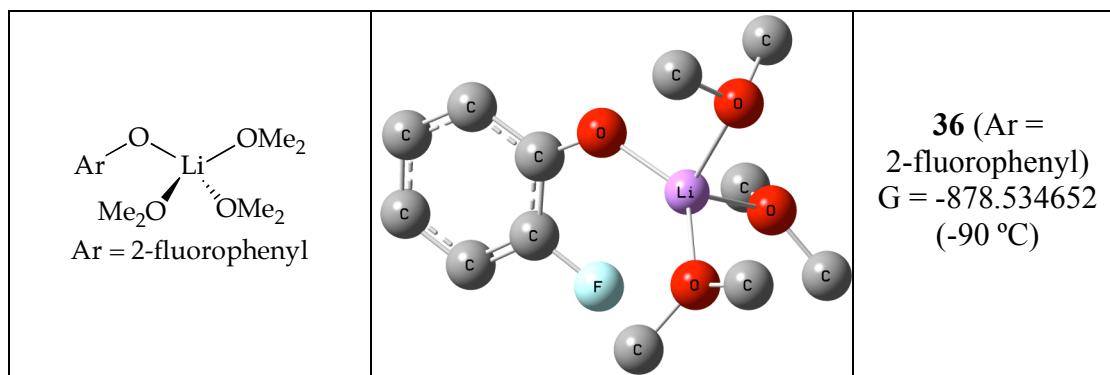
 <p>Ar = 2-fluorophenyl</p>		<p>35 (Ar = 2-fluorophenyl) G = -1447.181069 (-90 °C)</p>
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Atom	X	Y	Z	Atom	X	Y	Z
C	0.695895	-3.523938	2.026441	H	0.145633	2.006172	-3.324861
O	-0.077670	-2.349590	1.820078	H	-1.299534	1.337689	-2.507705
Li	0.074958	-1.145543	0.184386	C	0.465869	3.949277	-1.580878
O	1.385338	0.219345	-0.085941	H	-0.101780	4.747284	-2.080482
Li	-0.011512	1.456825	0.055137	H	0.736903	4.266131	-0.572587
O	-1.331795	0.167368	0.411193	H	1.377048	3.742271	-2.160359
C	-2.638971	0.094949	0.272894	C	2.693648	0.188236	-0.189335
C	-3.551142	0.374739	1.319505	C	3.499767	1.332138	-0.407776
C	-4.933493	0.286396	1.145120	C	4.890646	1.249660	-0.507082
C	-5.478216	-0.086137	-0.084950	C	5.547200	0.023358	-0.394893
C	-4.612950	-0.371506	-1.146878	C	4.786545	-1.133379	-0.182024
C	-3.246567	-0.279210	-0.950524	C	3.412047	-1.028380	-0.085519
F	-2.417025	-0.566016	-2.008591	F	2.673356	-2.166715	0.117183
H	-4.984543	-0.664066	-2.125207	H	5.248179	-2.112726	-0.090295
H	-6.553102	-0.154344	-0.223099	H	6.628290	-0.041346	-0.472790
H	-5.590754	0.510765	1.982275	H	5.465683	2.157392	-0.676393
H	-3.135701	0.663486	2.282501	H	2.997465	2.292012	-0.507858
O	0.275999	2.819982	1.554148	O	-0.094352	-2.605348	-1.208777
C	1.253832	2.484989	2.535266	C	-1.244325	-3.436415	-1.309073
H	0.858646	1.742024	3.242084	H	-0.969090	-4.431438	-1.688085
H	1.562131	3.381687	3.091426	H	-1.993947	-2.985435	-1.969230
H	2.109044	2.063764	2.005376	H	-1.656122	-3.530320	-0.302264
C	-0.909319	3.364216	2.123139	C	0.527329	-2.370199	-2.466385
H	-1.376877	2.650007	2.814061	H	0.884418	-3.313894	-2.903004
H	-1.596874	3.568846	1.300185	H	-0.174546	-1.890772	-3.161836
H	-0.687898	4.297244	2.660683	H	1.374464	-1.708729	-2.282732
O	-0.326995	2.777198	-1.447538	C	-0.443715	-1.706216	3.033829
C	-0.731777	2.245910	-2.707620	H	0.448994	-1.432830	3.615991
H	-1.361722	2.969887	-3.243308	H	-1.080904	-2.361797	3.644761

Table A1.5 (Continued).

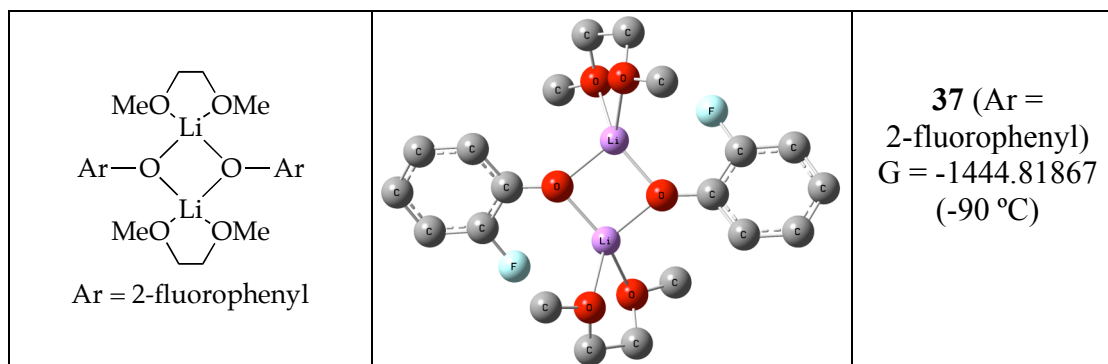
Atom	X	Y	Z
H	-0.994153	-0.808632	2.749695
H	1.642522	-3.287524	2.530501
H	0.135382	-4.252760	2.629712
H	0.907412	-3.941872	1.042099

Table A1.5 (Continued).



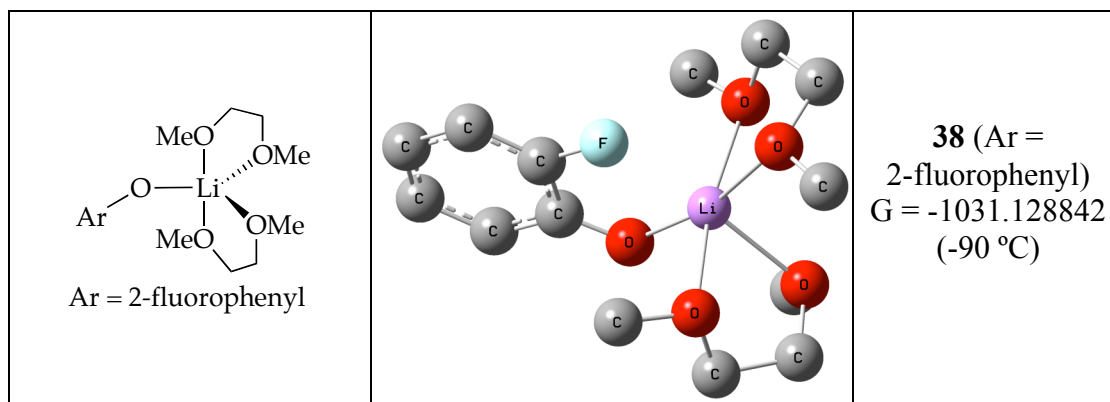
Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.962569	0.114765	0.022497	C	-2.238953	2.379044	1.232300
O	-1.364745	-0.798189	1.788717	H	-2.926702	3.236303	1.257435
C	-0.277365	-0.736816	2.713578	H	-2.522689	1.656720	1.999632
H	0.365084	-1.620114	2.613350	H	-1.211299	2.719561	1.408920
H	0.295083	0.155130	2.457610	C	-1.943707	2.561352	-1.101926
H	-0.656426	-0.671756	3.743098	H	-0.888088	2.836120	-1.003656
C	-2.141613	-1.976860	1.931839	H	-2.086001	1.995136	-2.025406
H	-1.529062	-2.874713	1.768337	H	-2.580615	3.456942	-1.124547
H	-2.592072	-2.029369	2.933498	O	0.556223	1.110044	0.052662
H	-2.933174	-1.938060	1.180707	C	1.792566	0.713014	-0.066947
O	-1.833120	-0.992263	-1.448195	C	2.140447	-0.662330	-0.105217
C	-3.181695	-0.825945	-1.865357	C	3.423736	-1.157133	-0.226947
H	-3.228330	-0.417098	-2.885054	C	4.489294	-0.253081	-0.318468
H	-3.717016	-1.786345	-1.846564	C	4.212020	1.116850	-0.284869
H	-3.646405	-0.124032	-1.171310	C	2.905794	1.589418	-0.162309
C	-1.086518	-1.837938	-2.320723	H	2.700451	2.657056	-0.136995
H	-1.037687	-1.405527	-3.329797	H	5.029424	1.831773	-0.355114
H	-0.085619	-1.920048	-1.899872	H	5.508063	-0.616663	-0.414315
H	-1.548916	-2.833558	-2.380141	H	3.580479	-2.232669	-0.246602
O	-2.328133	1.704994	-0.023001	F	1.088155	-1.563692	-0.013544

Table A1.5 (Continued).



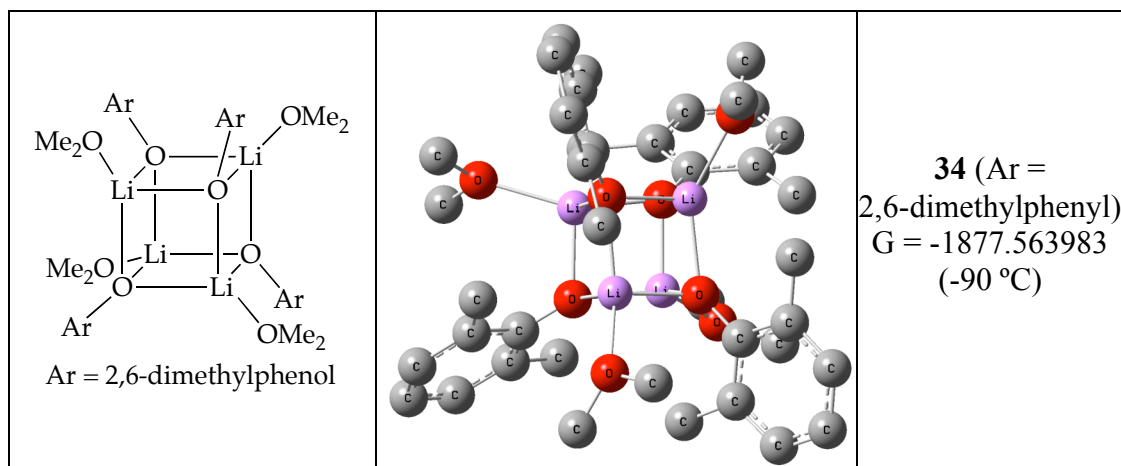
Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.306657	-1.263473	0.130257	H	-1.021266	3.448276	-2.962537
O	1.318826	-0.317157	0.291133	H	-1.035633	1.689633	-2.632222
Li	0.306608	1.263506	0.130246	C	2.616839	-0.490645	0.219713
O	-1.318886	0.317192	0.290934	C	3.296521	-1.620160	0.736658
C	-2.616908	0.490651	0.219602	C	4.682418	-1.758783	0.630310
C	-3.296567	1.620213	0.736473	C	5.458858	-0.778841	0.008689
C	-4.682474	1.758805	0.630216	C	4.825897	0.358504	-0.508592
C	-5.458948	0.778782	0.008766	C	3.453629	0.475172	-0.391692
C	-4.826010	-0.358614	-0.508432	F	2.835727	1.594778	-0.895718
C	-3.453732	-0.475250	-0.391622	H	5.384161	1.149973	-1.001297
F	-2.835856	-1.594911	-0.895557	H	6.536064	-0.888170	-0.073393
H	-5.384301	-1.150149	-1.001001	H	5.160799	-2.643508	1.044801
H	-6.536161	0.888087	-0.073247	H	2.700459	-2.377866	1.240722
H	-5.160835	2.643570	1.044644	O	0.033585	-2.788942	-1.252892
H	-2.700478	2.377986	1.240405	C	1.109325	-2.679988	-2.181498
O	-0.033531	2.789099	-1.252788	H	1.035523	-1.689311	-2.632315
C	-0.013543	4.026703	-0.555106	H	2.077257	-2.772832	-1.673746
C	1.126095	3.972450	0.442282	H	1.021358	-3.447944	-2.962686
O	0.892732	2.858197	1.298734	C	0.013766	-4.026574	-0.555253
C	1.935968	2.649047	2.247815	C	-1.125881	-3.972512	0.442135
H	2.014345	3.507617	2.929012	O	-0.892667	-2.858268	1.298640
H	1.671463	1.754356	2.813256	C	-1.935949	-2.649287	2.247708
H	2.896692	2.489000	1.743273	H	-2.014259	-3.507910	2.928845
H	2.084030	3.842982	-0.078542	H	-1.671548	-1.754610	2.813220
H	1.157389	4.905934	1.024474	H	-2.896674	-2.489303	1.743149
H	0.142813	4.863611	-1.253204	H	-1.157056	-4.906026	1.024286
H	-0.971542	4.181241	-0.035492	H	-2.083831	-3.843147	-0.078687
C	-1.109305	2.680305	-2.181372	H	0.971787	-4.180999	-0.035646
H	-2.077215	2.773244	-1.673594	H	-0.142478	-4.863478	-1.253380

Table A1.5 (Continued).



Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.693387	0.024169	0.079772	H	-1.452256	3.880155	0.648681
O	0.805444	-0.706814	0.969456	H	-0.384567	3.141532	-0.579576
C	1.987865	-0.429742	0.500144	C	0.378105	2.339241	1.813576
C	2.151864	0.358625	-0.670001	H	0.669656	1.469274	2.400527
C	3.358616	0.709012	-1.239813	H	0.146398	3.191608	2.468304
C	4.540061	0.263607	-0.631848	H	1.204293	2.606447	1.142342
C	4.448182	-0.518407	0.523978	O	-2.266748	-0.966267	1.266376
C	3.213712	-0.857684	1.077892	C	-2.520654	-2.239439	0.673652
H	3.155720	-1.466148	1.977451	C	-1.323490	-2.765709	-0.099896
H	5.358309	-0.871152	1.005132	O	-1.059135	-1.839054	-1.150276
H	5.504825	0.523692	-1.056855	C	0.054031	-2.227010	-1.951677
H	3.370195	1.317169	-2.140736	H	0.958775	-2.324527	-1.341312
F	0.972355	0.792054	-1.267154	H	-0.152934	-3.178620	-2.463066
O	-0.777244	1.954916	1.070387	H	0.203087	-1.438831	-2.691345
C	-1.193468	2.938976	0.137790	H	-0.438600	-2.844371	0.544766
C	-2.411806	2.402172	-0.583280	H	-1.561115	-3.758320	-0.517098
O	-2.049429	1.177502	-1.203639	H	-2.822113	-2.966629	1.440933
C	-3.120192	0.581247	-1.920963	H	-3.362027	-2.097986	-0.013535
H	-2.750628	-0.372764	-2.296217	C	-1.764454	-1.035577	2.606028
H	-3.984526	0.406111	-1.263523	H	-0.754030	-1.454676	2.627888
H	-3.432866	1.221697	-2.758554	H	-2.448517	-1.621219	3.236238
H	-3.233639	2.233378	0.129598	H	-1.728684	-0.007011	2.969255
H	-2.749142	3.132062	-1.336158				

Table A1.5 (Continued).

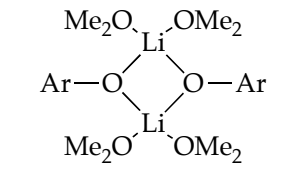
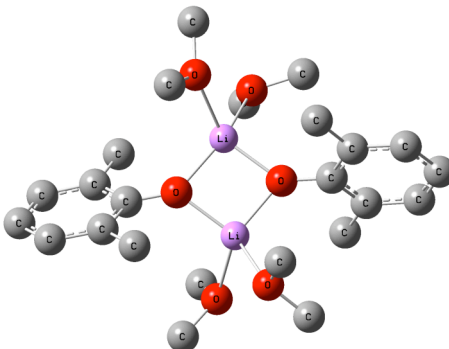


Atom	X	Y	Z	Atom	X	Y	Z
O	1.477324	-0.265196	1.017951	H	-1.020415	5.813166	-1.540146
Li	1.309959	-0.313251	-0.949540	H	0.212759	6.018435	-3.690344
O	-0.266862	-1.475763	-1.015106	H	1.442634	4.041298	-4.573922
Li	-1.306956	0.317607	-0.955298	C	1.644386	1.570131	-3.514058
O	-1.481266	0.266035	1.011929	H	2.105634	1.819850	-4.475736
Li	-0.315671	-1.308187	0.953249	H	2.433966	1.190107	-2.855913
O	-1.383369	-2.841583	2.083747	H	0.949583	0.737057	-3.688209
C	-1.880849	-2.610263	3.401667	O	1.378645	2.840123	2.091960
H	-1.783415	-3.521065	4.009527	C	2.062710	3.929887	1.474851
H	-1.281575	-1.816200	3.845578	H	3.140989	3.731121	1.428268
H	-2.929532	-2.293666	3.370613	H	1.666792	4.042184	0.464915
C	-2.066796	-3.928369	1.460536	H	1.892776	4.857095	2.040528
H	-1.665699	-4.039380	0.452520	C	1.870636	2.606199	3.411390
H	-1.901994	-4.857147	2.025132	H	2.921231	2.295685	3.384362
H	-3.144298	-3.726910	1.408767	H	1.765023	3.513833	4.022654
Li	0.311773	1.308761	0.956694	H	1.273935	1.806736	3.848957
O	0.270616	1.479524	-1.010274	C	-2.643570	0.245167	1.687755
C	0.250462	2.640284	-1.688718	C	-2.766774	0.922266	2.931855
C	0.931284	2.761537	-2.931104	C	-3.979997	0.899518	3.625384
C	0.910400	3.973667	-3.626658	C	-5.088358	0.211997	3.133612
C	0.220973	5.082486	-3.138633	C	-4.966649	-0.469860	1.924480
C	-0.464975	4.962276	-1.931617	C	-3.771959	-0.470993	1.193770
C	-0.467748	3.768922	-1.198828	C	-3.703557	-1.235120	-0.108205
C	-1.237200	3.700927	0.099988	H	-3.766167	-0.575560	-0.982474
H	-1.944179	4.534688	0.174989	H	-2.772777	-1.799434	-0.210819
H	-1.801117	2.769494	0.199956	H	-4.538064	-1.940844	-0.186671
H	-0.580648	3.764649	0.976663	H	-5.817245	-1.023348	1.529655

Table A1.5 (Continued).

Atom	X	Y	Z	Atom	X	Y	Z
H	-6.025035	0.202399	3.684051	H	-2.102664	-1.819946	-4.479929
H	-4.048924	1.428477	4.574383	H	-2.426704	-1.185809	-2.861093
C	-1.575628	1.630620	3.520631	O	2.832786	-1.394728	-2.081059
H	-1.828343	2.092336	4.481285	C	2.607561	-1.874833	-3.406045
H	-0.746857	0.931513	3.698796	H	2.345486	-2.938941	-3.393512
H	-1.188241	2.418811	2.865224	H	1.776004	-1.309456	-3.824662
O	-2.821646	1.403505	-2.078705	H	3.502781	-1.718657	-4.024721
C	-3.930825	2.069185	-1.476730	C	3.937250	-2.062430	-1.473074
H	-3.758446	3.152663	-1.445608	H	4.859869	-1.870458	-2.039325
H	-4.851583	1.868127	-2.042839	H	4.044738	-1.672853	-0.460143
H	-4.038055	1.686425	-0.461146	H	3.758598	-3.144721	-1.435082
C	-2.596749	1.874786	-3.406820	C	2.638895	-0.247740	1.695141
H	-1.747106	1.326715	-3.811773	C	2.759926	-0.927172	2.938133
H	-3.482226	1.690024	-4.031686	C	3.973224	-0.908802	3.631738
H	-2.361890	2.945420	-3.403622	C	5.083428	-0.223344	3.141265
C	-0.246622	-2.637110	-1.692625	C	4.963538	0.461582	1.933652
C	-0.926450	-2.759056	-2.935450	C	3.768717	0.467515	1.203253
C	-0.905302	-3.971705	-3.630096	C	3.700544	1.235037	-0.096732
C	-0.216870	-5.080472	-3.140581	H	4.541139	1.933084	-0.178616
C	0.468020	-4.959632	-1.933026	H	3.751614	0.576262	-0.972309
C	0.470785	-3.765661	-1.201240	H	2.774344	1.807822	-0.193031
C	1.240272	-3.696740	0.097502	H	5.815544	1.013729	1.540019
H	1.807517	-2.767115	0.194624	H	6.020204	-0.217598	3.691587
H	0.584736	-3.755635	0.975284	H	4.040710	-1.439608	4.579804
H	1.944475	-4.532681	0.174405	C	1.566747	-1.633303	3.525536
H	1.022753	-5.810434	-1.540392	H	0.739169	-0.932602	3.702947
H	-0.208542	-6.016834	-3.691585	H	1.178243	-2.420499	2.869620
H	-1.436636	-4.039866	-4.577836	H	1.817597	-2.095776	4.486323
C	-1.638889	-1.568042	-3.520042				
H	-0.943552	-0.736351	-3.698291				

Table A1.5 (Continued).

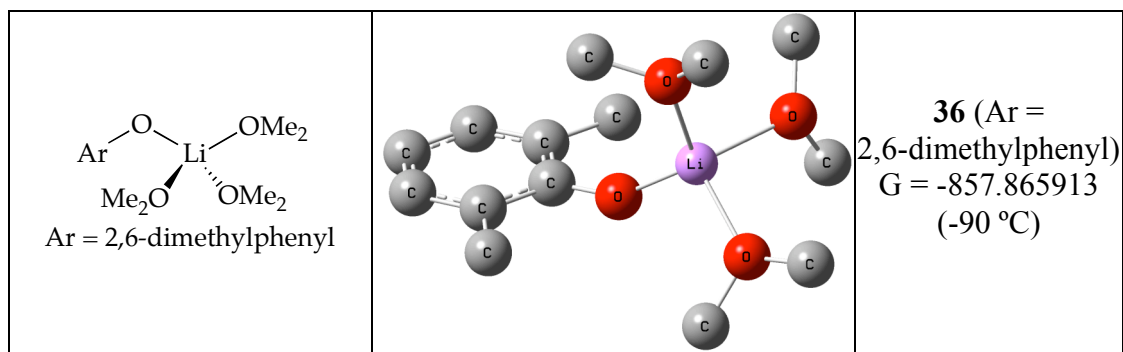
 <p>Ar = 2,6-dimethylphenyl</p>		<p>35 (Ar = 2,6-dimethylphenyl) G = -1405.835621 (-90 °C)</p>
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Atom	X	Y	Z	Atom	X	Y	Z
C	1.789011	-3.408701	1.270354	H	-2.791193	2.257589	1.593193
O	0.801830	-2.446600	1.639699	H	-2.340257	3.010479	0.048577
Li	0.071547	-1.232035	0.070917	H	-2.528769	4.031659	1.506489
O	1.430031	0.069257	-0.159048	O	0.516945	2.799151	-1.382577
Li	0.039086	1.362430	0.013282	C	0.390579	4.212812	-1.345969
O	-1.313776	0.046559	0.066252	H	1.376864	4.693478	-1.416675
C	-2.627662	-0.085473	-0.049038	H	-0.239239	4.573223	-2.172497
C	-3.400925	-0.611176	1.025803	H	-0.068773	4.464937	-0.389948
C	-4.785161	-0.748796	0.883948	C	1.173935	2.335950	-2.558878
C	-5.438470	-0.378577	-0.292063	H	2.171631	2.786906	-2.646760
C	-4.685346	0.149613	-1.341370	H	1.274649	1.256288	-2.453225
C	-3.299734	0.307690	-1.242598	H	0.584888	2.580688	-3.454209
C	-2.507130	0.898469	-2.383442	C	2.755423	-0.001132	-0.176118
H	-1.954075	1.797029	-2.079716	C	3.542016	0.788628	0.710763
H	-1.751235	0.200096	-2.765173	C	4.935081	0.681797	0.694277
H	-3.164571	1.171588	-3.216460	C	5.590264	-0.179832	-0.185216
H	-5.182387	0.452004	-2.262266	C	4.826190	-0.938884	-1.071858
H	-6.514961	-0.492784	-0.386516	C	3.430364	-0.864101	-1.087757
H	-5.360188	-1.150641	1.717246	C	2.632773	-1.673197	-2.080994
C	-2.711850	-0.992107	2.313005	H	3.294464	-2.254806	-2.732465
H	-2.142970	-0.149057	2.728811	H	1.944958	-2.376381	-1.594084
H	-3.437469	-1.316677	3.067126	H	2.013465	-1.031043	-2.722556
H	-1.987792	-1.805405	2.172515	H	5.321863	-1.604972	-1.776933
O	-0.804339	2.871967	1.383188	H	6.674494	-0.251691	-0.186235
C	-0.519129	2.912572	2.774617	H	5.515453	1.291225	1.385773
H	-1.027580	2.094719	3.305220	C	2.853967	1.742715	1.653603
H	-0.839835	3.870501	3.209302	H	3.578924	2.259856	2.292145
H	0.560038	2.807388	2.890109	H	2.283823	2.507685	1.108090
C	-2.197539	3.053313	1.128907	H	2.138429	1.223010	2.304758

Table A1.5 (Continued).

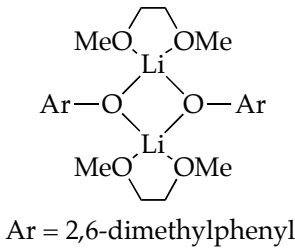
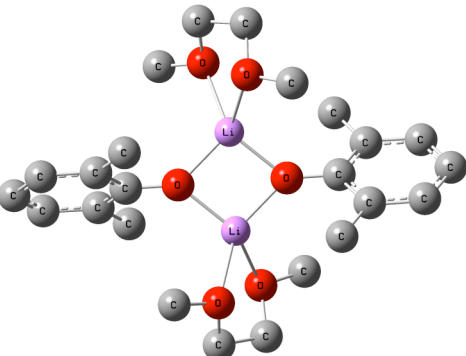
Atom	X	Y	Z
O	-0.659246	-2.908888	-0.965107
C	-1.584698	-3.722772	-0.244192
H	-1.683881	-4.706313	-0.725073
H	-2.568417	-3.239265	-0.191291
H	-1.182148	-3.844810	0.762089
C	-1.090414	-2.686464	-2.305306
H	-1.157011	-3.639204	-2.849756
H	-2.066756	-2.186582	-2.320192
H	-0.343138	-2.050276	-2.782469
C	1.189773	-1.713929	2.798277
H	2.139127	-1.191099	2.627952
H	1.291962	-2.387667	3.661200
H	0.399600	-0.987920	2.997696
H	2.737913	-2.916579	1.021855
H	1.949738	-4.126666	2.087208
H	1.408990	-3.933753	0.392766

Table A1.5 (Continued).



Atom	X	Y	Z	Atom	X	Y	Z
Li	1.161651	-0.021204	-0.014584	H	1.522711	2.830959	-1.586953
O	2.311890	-1.160157	-1.233425	C	2.239428	2.634280	0.955519
C	1.577719	-1.932630	-2.186074	H	1.367693	3.283346	0.798248
H	1.665527	-3.005088	-1.962413	H	2.124613	2.096887	1.898070
H	0.540616	-1.607204	-2.092156	H	3.148479	3.251575	0.986593
H	1.956034	-1.744638	-3.200966	O	-0.494445	-0.097924	-0.632936
C	3.694531	-1.465132	-1.207887	C	-1.787409	-0.002875	-0.406185
H	3.866205	-2.509763	-0.909398	C	-2.584837	-1.170244	-0.207262
H	4.152864	-1.301992	-2.194351	C	-3.953708	-1.046691	0.041877
H	4.161563	-0.795901	-0.481425	C	-4.577943	0.200495	0.096449
O	1.320985	-0.491468	1.961537	C	-3.805879	1.345701	-0.107828
C	2.454014	-1.010829	2.638125	C	-2.434223	1.268134	-0.355794
H	2.532456	-0.593491	3.652485	C	-1.614846	2.510012	-0.594357
H	2.404643	-2.106896	2.709678	H	-0.799451	2.605307	0.136860
H	3.337894	-0.724297	2.063323	H	-2.233118	3.412810	-0.530575
C	0.094168	-0.777119	2.637928	H	-1.137223	2.491903	-1.583941
H	0.080184	-0.287942	3.621890	H	-4.278382	2.327241	-0.075716
H	-0.712903	-0.396399	2.012378	H	-5.644645	0.278563	0.290086
H	-0.028682	-1.860268	2.772341	H	-4.542752	-1.951228	0.192028
O	2.334417	1.652597	-0.070787	C	-1.931062	-2.526262	-0.293489
C	2.415717	2.230681	-1.371659	H	-1.546066	-2.727601	-1.303154
H	3.312103	2.860898	-1.458466	H	-2.639950	-3.324078	-0.043717
H	2.476260	1.402885	-2.079592	H	-1.068409	-2.611488	0.381303

Table A1.5 (Continued).

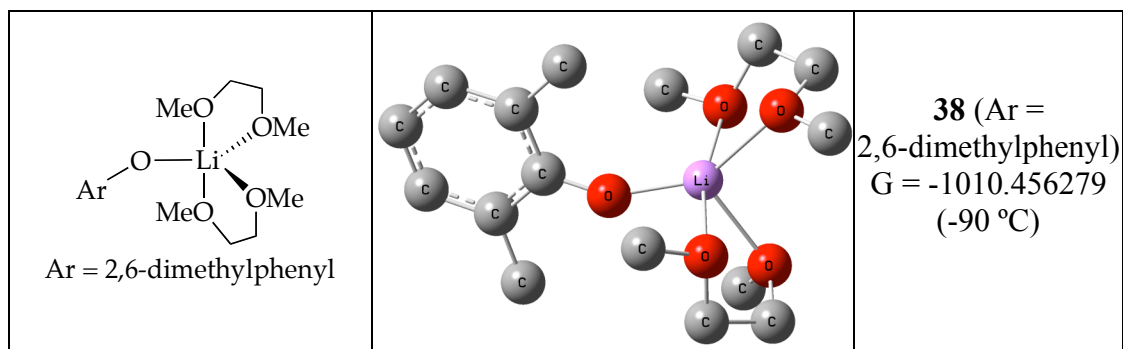
 <p>Ar = 2,6-dimethylphenyl</p>		<p>37 (Ar = 2,6-dimethylphenyl) G = -1403.482645 (-90 °C)</p>
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Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.000105	1.264150	0.000152	H	1.531669	-4.087760	0.136210
O	1.380002	0.000087	0.000124	H	0.585857	-4.958286	-1.103507
Li	-0.000012	-1.264069	-0.000007	H	-0.585656	-4.958054	1.104527
O	-1.380125	-0.000008	-0.000020	H	-1.531473	-4.087807	-0.135380
C	-2.707710	-0.000058	-0.000133	C	-1.669153	-2.724919	2.104970
C	-3.433432	-0.607438	-1.063893	H	-2.600839	-2.642593	1.532151
C	-4.831069	-0.595210	-1.043836	H	-1.731662	-3.570973	2.803108
C	-5.541174	-0.000224	-0.000351	H	-1.509194	-1.801109	2.660853
C	-4.831299	0.594863	1.043234	C	2.707587	0.000036	-0.000074
C	-3.433667	0.607265	1.063500	C	3.433291	0.607108	-1.064023
C	-2.680868	1.243742	2.205910	C	4.830928	0.594766	-1.044056
H	-2.019941	0.524937	2.709297	C	5.541052	-0.000033	-0.000477
H	-2.028199	2.061086	1.872414	C	4.831195	-0.594808	1.043298
H	-3.371293	1.648546	2.954287	C	3.433563	-0.607089	1.063661
H	-5.371425	1.061041	1.866384	C	2.680790	-1.243208	2.206287
H	-6.627947	-0.000290	-0.000434	H	3.371237	-1.647896	2.954707
H	-5.371013	-1.061435	-1.867079	H	2.019979	-0.524210	2.709550
C	-2.680380	-1.243787	-2.206207	H	2.028003	-2.060560	1.873046
H	-2.019189	-0.524971	-2.709229	H	5.371336	-1.060828	1.866528
H	-2.027933	-2.061303	-1.872690	H	6.627825	-0.000059	-0.000632
H	-3.370635	-1.648336	-2.954879	H	5.370858	1.060750	-1.867446
O	-0.548089	-2.880475	1.235577	C	2.680220	1.243254	-2.206438
C	-0.604027	-4.068237	0.456937	H	3.370463	1.647552	-2.955256
C	0.604222	-4.068331	-0.456109	H	2.018920	0.524384	-2.709237
O	0.548275	-2.880738	-1.235009	H	2.027876	2.060912	-1.873071
C	1.669317	-2.725395	-2.104471	O	0.548212	2.880767	1.235483
H	1.731796	-3.571612	-2.802414	C	1.669245	2.725160	2.104908
H	1.509357	-1.801714	-2.660570	H	1.509013	1.801591	2.661114
H	2.601018	-2.642949	-1.531694	H	2.600895	2.642354	1.532098

Table A1.5 (Continued).

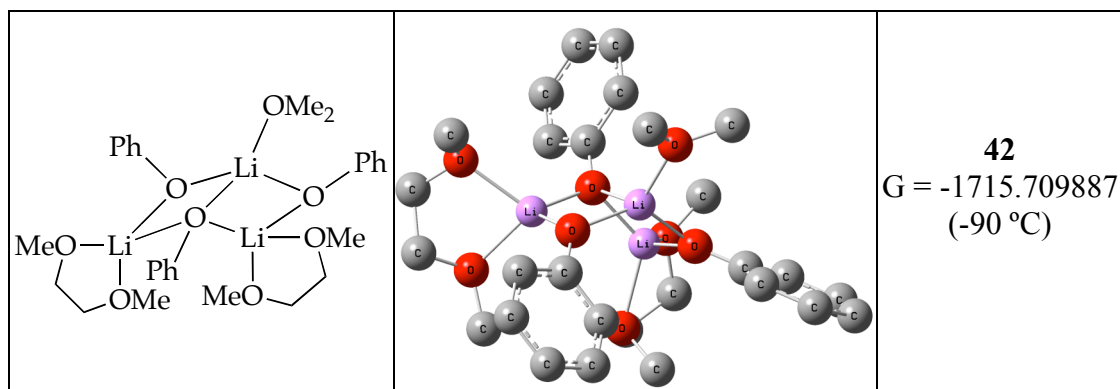
Atom	X	Y	Z
H	1.732027	3.571431	2.802759
C	0.604488	4.068281	0.456488
C	-0.603803	4.068488	-0.456502
O	-0.548273	2.880640	-1.235035
C	-1.669433	2.725329	-2.104348
H	-1.731692	3.571296	-2.802612
H	-1.509826	1.801373	-2.660088
H	-2.601116	2.643411	-1.531464
H	-0.585184	4.958241	-1.104173
H	-1.531216	4.088401	0.135856
H	1.531913	4.087380	-0.135876
H	0.586428	4.958296	1.103815

Table A1.5 (Continued).



Atom	X	Y	Z	Atom	X	Y	Z
Li	1.007765	0.065022	-0.008274	H	4.034853	1.802107	2.060908
O	-0.708989	-0.430986	0.065006	H	3.481048	1.991821	-0.986644
C	-1.991086	-0.167000	0.162496	H	3.280923	3.276985	0.238082
C	-2.474892	0.859049	1.032199	H	1.720957	3.606229	-1.671819
C	-3.844252	1.122635	1.110826	H	0.837338	3.316532	-0.149063
C	-4.773344	0.402959	0.357916	C	-0.402230	1.983005	-2.009867
C	-4.309537	-0.606375	-0.488172	H	-0.806622	1.031393	-2.351778
C	-2.949838	-0.901464	-0.599966	H	-0.312588	2.685222	-2.850974
C	-2.466776	-1.997825	-1.514734	H	-1.078285	2.394168	-1.251260
H	-3.306348	-2.510740	-1.997775	O	2.219863	-1.221806	-1.205231
H	-1.810090	-1.611607	-2.307636	C	2.608343	-2.377579	-0.456435
H	-1.878478	-2.748924	-0.969444	C	1.615441	-2.687318	0.649451
H	-5.021014	-1.182258	-1.079795	O	1.633608	-1.588392	1.551857
H	-5.835752	0.619639	0.433023	C	0.668770	-1.730311	2.594180
H	-4.188676	1.909741	1.781490	H	-0.342290	-1.734329	2.175651
C	-1.489615	1.637400	1.867236	H	0.856129	-2.649634	3.168500
H	-1.999302	2.378308	2.493827	H	0.785157	-0.866618	3.252816
H	-0.905547	0.981750	2.527181	H	0.602374	-2.813554	0.243597
H	-0.753870	2.172187	1.249118	H	1.911895	-3.615350	1.166514
O	0.885664	1.709509	-1.455369	H	2.721905	-3.243584	-1.122063
C	1.502591	2.855920	-0.895161	H	3.585484	-2.151765	-0.016001
C	2.792666	2.413235	-0.238505	C	1.508150	-1.522673	-2.407933
O	2.476260	1.423306	0.733884	H	0.562846	-2.034572	-2.197185
C	3.618011	0.981801	1.459944	H	2.129756	-2.136702	-3.074004
H	3.286193	0.170089	2.106240	H	1.298531	-0.564931	-2.885935
H	4.394524	0.607517	0.777218				

Table A1.5 (Continued).

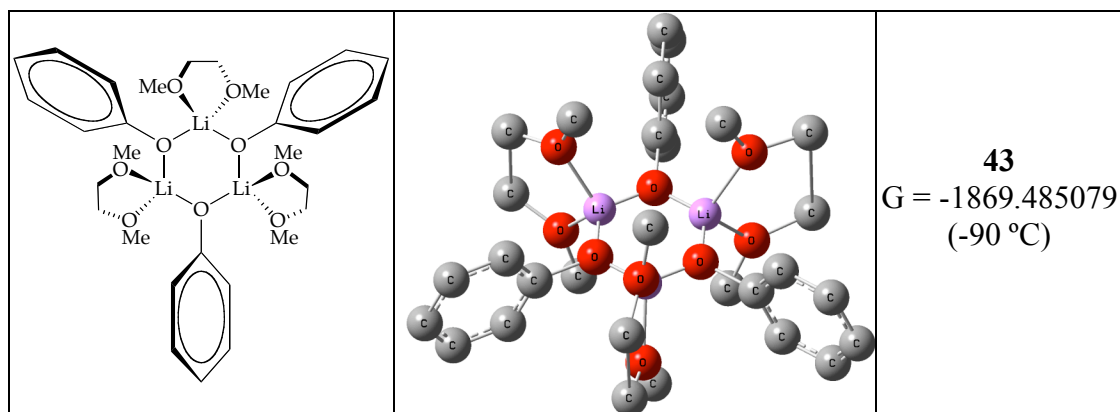


Atom	X	Y	Z	Atom	X	Y	Z
O	-0.362622	1.356205	0.261324	H	-0.417936	-5.146114	-1.361129
Li	1.192905	0.898882	-0.747318	H	-2.731934	-6.041634	-1.101597
O	1.838030	-0.482937	0.292522	H	-4.456857	-4.631303	0.018359
Li	0.147311	-0.440884	1.155202	H	-3.879349	-2.374198	0.857100
O	-1.525389	-1.215285	0.621335	O	0.322252	-0.688748	3.123277
Li	-1.976241	0.440570	-0.089876	C	-0.702566	-1.352063	3.852374
O	-2.870056	0.400431	-1.954577	H	-0.370939	-2.351357	4.168260
C	-4.276735	0.405075	-1.734291	H	-1.549590	-1.446689	3.171506
C	-4.546372	1.493978	-0.708021	H	-0.986762	-0.770926	4.741830
O	-3.797201	1.247357	0.484449	C	1.541342	-0.563655	3.843520
C	-4.530176	0.607226	1.526673	H	1.399026	0.050591	4.744650
H	-3.816760	0.392200	2.323149	H	2.257861	-0.084762	3.174852
H	-5.315955	1.274490	1.904792	H	1.925769	-1.550206	4.135650
H	-4.980400	-0.334459	1.187675	C	2.933254	-1.217776	0.389319
H	-4.203969	2.458493	-1.096325	C	4.204600	-0.708717	0.018875
H	-5.619254	1.565470	-0.487468	C	5.358400	-1.485544	0.116738
H	-4.813069	0.624460	-2.670819	C	5.299100	-2.799708	0.587176
H	-4.602200	-0.580214	-1.368165	C	4.055990	-3.319971	0.961143
C	-2.436852	-0.591962	-2.888382	C	2.896619	-2.552848	0.866961
H	-1.359144	-0.460613	-2.999195	H	1.934422	-2.972437	1.151538
H	-2.651474	-1.599787	-2.514055	H	3.986620	-4.342050	1.329254
H	-2.928265	-0.439514	-3.859312	H	6.199288	-3.403347	0.663124
C	-1.825385	-2.435573	0.199589	H	6.316183	-1.056540	-0.173475
C	-3.128695	-2.974835	0.347590	H	4.261376	0.320921	-0.329661
C	-3.445548	-4.251381	-0.117280	O	2.313047	2.434489	-1.474729
C	-2.482433	-5.046781	-0.743075	C	2.874594	2.076544	-2.731355
C	-1.187127	-4.539297	-0.886633	C	1.770297	1.380019	-3.514533
C	-0.859912	-3.264359	-0.428983	O	1.217275	0.285750	-2.783424
H	0.152051	-2.880738	-0.535768	C	1.902956	-0.961115	-2.967652

Table A1.5 (Continued).

Atom	X	Y	Z
H	2.928893	-0.923600	-2.585534
H	1.346019	-1.704379	-2.397688
H	1.905895	-1.230961	-4.032234
H	2.143776	1.045548	-4.492354
H	0.945634	2.081747	-3.674050
H	3.204952	2.974237	-3.275977
H	3.746327	1.421331	-2.583606
C	3.153117	3.248564	-0.659535
H	3.391643	4.188090	-1.175270
H	2.589105	3.464611	0.248934
H	4.083609	2.723256	-0.405749
C	-0.366885	2.624934	0.693490
C	0.089385	2.960634	1.988343
C	0.097658	4.285866	2.425772
C	-0.346089	5.318309	1.595105
C	-0.802238	5.000915	0.312644
C	-0.813201	3.680095	-0.135412
H	-1.160937	3.437537	-1.137502
H	-1.152490	5.790956	-0.348943
H	-0.338531	6.348439	1.940529
H	0.453066	4.512345	3.429146
H	0.427086	2.157863	2.639112

Table A1.5 (Continued).

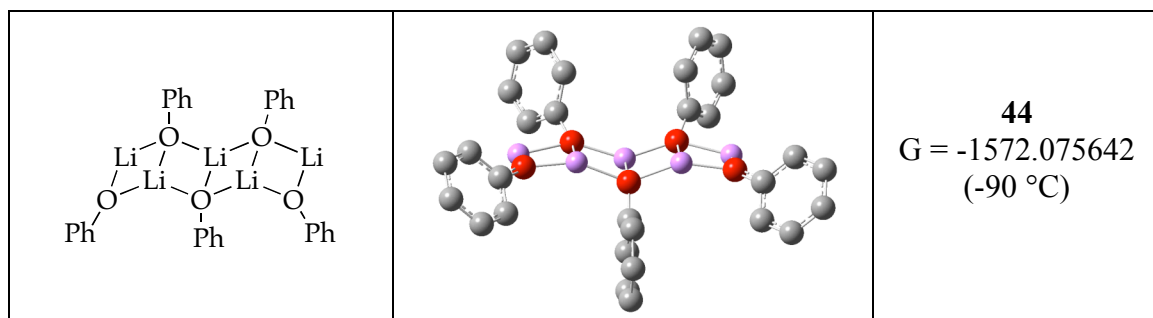


Atom	X	Y	Z	Atom	X	Y	Z
Li	-3.018404	1.912134	-0.001678	C	-7.348989	0.703398	1.206322
Li	-0.925925	0.703703	0.000000	H	-5.404546	0.701421	2.159293
Li	-3.018623	-0.504047	0.000000	C	-7.348199	0.706405	-1.209858
C	-0.853911	-1.837983	0.001841	H	-5.402949	0.707226	-2.161619
C	-0.505715	-2.440833	1.210375	C	-8.046085	0.705576	-0.001816
C	-0.504575	-2.443442	-1.205883	H	-7.898973	0.702410	2.158508
C	0.190762	-3.649711	1.211942	H	-7.898096	0.707707	-2.162268
H	-0.781192	-1.964126	2.162270	H	-9.145689	0.706214	-0.002259
C	0.192150	-3.651792	-1.204238	O	-1.623579	1.912212	-0.001199
H	-0.779172	-1.967900	-2.158643	O	-3.716005	0.703928	-0.000682
C	0.539514	-4.255192	0.004750	O	-1.623463	-0.504047	0.000000
H	0.464800	-4.125067	2.164876	C	1.768816	0.704332	1.479852
H	0.467619	-4.129211	-2.155901	C	1.771354	0.702866	-1.475220
H	1.088603	-5.207888	0.005802	C	-0.397071	0.701984	-3.028516
C	-0.853075	3.245600	-0.001281	C	-0.402275	0.704990	3.029420
C	-0.501975	3.848365	-1.209016	H	0.374056	0.670780	-3.769656
C	-0.505783	3.850647	1.207239	H	-1.027799	-0.155928	-3.133717
C	0.195364	5.056748	-1.208992	H	-0.979238	1.590547	-3.156721
H	-0.775840	3.371984	-2.161540	H	-0.590764	1.712935	3.335065
C	0.191804	5.058500	1.207187	H	-1.324064	0.162365	3.001794
H	-0.782669	3.375171	2.159370	H	0.264560	0.240084	3.725187
C	0.542074	5.661817	-0.001005	H	2.209075	-0.184833	1.880421
H	0.471692	5.532037	-2.161297	H	2.209063	1.593901	1.879539
H	0.465663	5.535594	2.159477	H	2.212301	-0.186696	-1.874149
H	1.091842	6.614121	-0.000802	H	2.212288	1.592038	-1.875031
C	-5.256005	0.704184	-0.000934	O	0.238743	0.702780	-1.625897
C	-5.953829	0.702361	1.206650	O	0.235948	0.704395	1.627896
C	-5.953374	0.705847	-1.209607	O	-3.568283	-1.456924	-1.536879

Table A1.5 (Continued).

Atom	X	Y	Z
O	-3.568283	-1.455188	1.537954
C	-4.430106	-2.530484	-1.150056
C	-4.450174	-2.513651	1.154777
H	-4.044679	-3.461690	-1.509500
H	-5.417156	-2.367091	-1.529444
H	-4.093605	-3.448198	1.534752
H	-5.439006	-2.320013	1.514799
C	-3.181949	-1.151456	-2.879390
C	-3.164563	-1.161660	2.878010
H	-2.394700	-0.426882	-2.867887
H	-4.022271	-0.756702	-3.411299
H	-2.839800	-2.042216	-3.363518
H	-2.152904	-1.478453	3.023223
H	-3.802259	-1.678960	3.564046
H	-3.236443	-0.107935	3.049462
O	-3.568595	2.865717	1.534573
O	-3.567539	2.862573	-1.540254
C	-4.249413	4.056093	-1.145975
C	-4.247663	4.059876	1.137395
H	-3.726209	4.919339	1.503876
H	-5.251965	4.052572	1.506481
H	-3.730983	4.915825	-1.516099
H	-5.254253	4.044699	-1.513489
C	-3.340934	2.456232	2.885644
C	-3.336755	2.451579	-2.890337
H	-2.323420	2.664759	-3.159793
H	-3.998451	2.982094	-3.542727
H	-3.515710	1.400356	-2.978692
H	-2.753115	1.562189	2.893129
H	-4.279342	2.270118	3.364865
H	-2.819998	3.229991	3.409880

Table A1.5 (Continued).

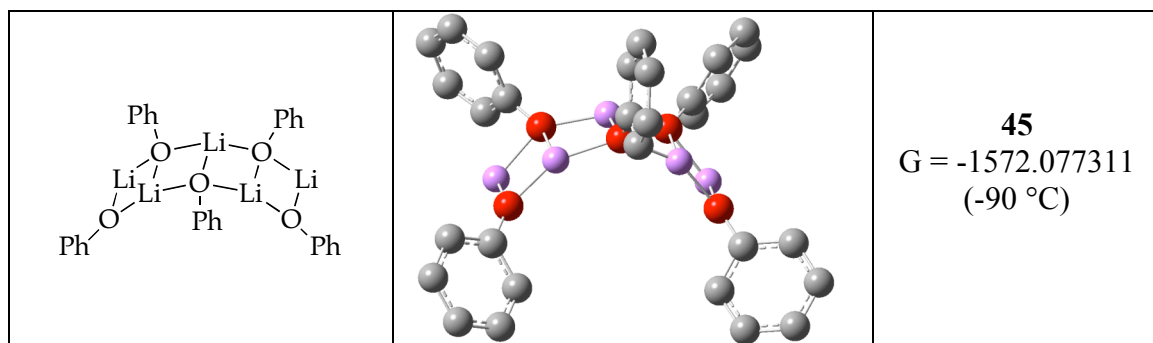


Atom	X	Y	Z	Atom	X	Y	Z
O	-1.734417	1.530442	0.507754	H	5.623158	-0.291765	-1.806892
Li	0.016209	1.029169	0.896421	C	2.312203	2.682878	0.403991
O	-0.019135	-0.791315	0.249190	C	3.154090	3.248638	1.389137
Li	-1.780508	-0.347128	-0.274300	C	3.757589	4.495777	1.186961
O	-3.591463	-0.527469	-0.180613	C	3.534151	5.203269	0.008054
Li	-3.575408	1.037540	0.629129	C	2.697806	4.652970	-0.971047
C	-4.496453	-1.458987	-0.525589	C	2.098056	3.410325	-0.786176
C	-5.527452	-1.161285	-1.439666	H	1.460575	2.978983	-1.553154
C	-6.469533	-2.127991	-1.791953	H	2.516290	5.197935	-1.894050
C	-6.409970	-3.412776	-1.247363	H	3.998679	6.171992	-0.148940
C	-5.389174	-3.717916	-0.343407	H	4.391120	4.914254	1.964910
C	-4.443182	-2.758778	0.017112	H	3.276151	2.724430	2.337991
H	-3.651197	-2.997012	0.723131	C	-0.038968	-1.993261	0.890751
H	-5.327271	-4.714215	0.088974	C	-0.055765	-3.195606	0.159972
H	-7.144646	-4.163772	-1.524116	C	-0.076722	-4.425528	0.819375
H	-7.254644	-1.873649	-2.500732	C	-0.081093	-4.485680	2.214707
H	-5.565745	-0.164026	-1.873744	C	-0.064317	-3.296683	2.947160
Li	1.761747	-0.408743	-0.257028	C	-0.043411	-2.062487	2.296585
O	1.806375	1.445104	0.588126	H	-0.030205	-1.137845	2.871314
Li	3.631995	0.863249	0.650745	H	-0.067492	-3.326492	4.034029
O	3.564382	-0.667794	-0.219382	H	-0.097558	-5.444757	2.723983
C	4.409227	-1.627459	-0.631461	H	-0.090230	-5.341723	0.234607
C	5.493678	-1.321340	-1.478466	H	-0.052401	-3.149667	-0.926788
C	6.372435	-2.318702	-1.901648	C	-2.175138	2.774435	0.219844
C	6.194973	-3.643595	-1.496820	C	-2.911462	3.499165	1.184221
C	5.120549	-3.957147	-0.660432	C	-3.448521	4.755391	0.879744
C	4.237405	-2.967621	-0.229594	C	-3.264410	5.313955	-0.383464
H	3.404733	-3.213541	0.425212	C	-2.534561	4.604222	-1.344371
H	4.967092	-4.984113	-0.336093	C	-1.999826	3.351226	-1.056165
H	6.880490	-4.418342	-1.828733	H	-1.445096	2.795615	-1.807884
H	7.200651	-2.056493	-2.556468	H	-2.385663	5.030603	-2.333293

Table A1.5 (Continued).

Atom	X	Y	Z
H	-3.678947	6.289265	-0.619676
H	-4.001469	5.297957	1.642349
H	-3.007650	3.085916	2.188611

Table A1.5 (Continued).

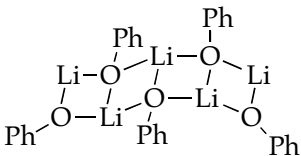
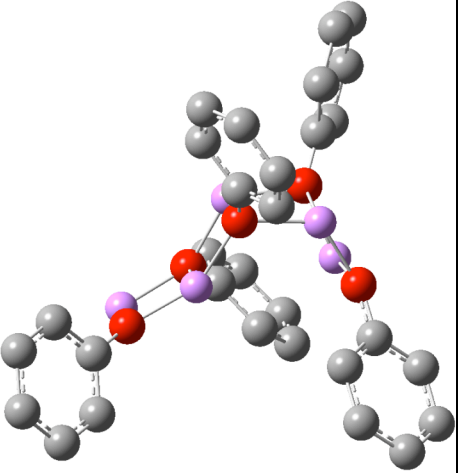


Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.000653	1.556974	0.129381	C	0.001793	-0.395068	2.464451
O	-1.771208	1.557245	-0.460087	C	0.002425	-1.736321	2.896866
Li	-1.728224	-0.304600	0.410940	C	0.003539	-2.041607	4.258947
O	0.000738	-0.098846	1.138327	C	0.004042	-1.025535	5.217429
Li	1.728544	-0.303623	0.407961	C	0.003402	0.306412	4.797375
O	1.769005	1.557665	-0.463503	C	0.002302	0.623261	3.438161
Li	2.965986	0.557787	-1.528135	H	0.001801	1.662796	3.114883
O	2.943323	-1.021245	-0.749065	H	0.003766	1.108665	5.531332
C	3.514425	-2.228982	-0.898966	H	0.004916	-1.267970	6.276043
C	4.812491	-2.481059	-0.411404	H	0.004030	-3.083329	4.569600
C	5.400995	-3.735807	-0.569680	H	0.002083	-2.527527	2.150388
C	4.717070	-4.768704	-1.215212	O	-2.943657	-1.022711	-0.745062
C	3.430062	-4.528035	-1.702007	Li	-2.968935	0.556873	-1.523176
C	2.832624	-3.276875	-1.549479	C	-3.515032	-2.230153	-0.896316
H	1.830767	-3.088151	-1.928879	C	-4.813142	-2.482483	-0.408996
H	2.882882	-5.321514	-2.206264	C	-5.401949	-3.736902	-0.568788
H	5.178521	-5.744825	-1.335543	C	-4.718305	-4.769164	-1.215621
H	6.403433	-3.906475	-0.183261	C	-3.431242	-4.528247	-1.702158
H	5.342462	-1.677018	0.094643	C	-2.833493	-3.277425	-1.548118
C	2.589404	2.625748	-0.553808	H	-1.831589	-3.088445	-1.927257
C	3.198647	3.195060	0.585104	H	-2.884265	-5.321257	-2.207366
C	4.093315	4.253866	0.451334	H	-5.180031	-5.745011	-1.337112
C	4.416547	4.769193	-0.809704	H	-6.404423	-3.907824	-0.182573
C	3.823048	4.216426	-1.942682	H	-5.342850	-1.678927	0.098090
C	2.915341	3.158084	-1.821790	C	-2.591285	2.625540	-0.551446
H	2.400990	2.769737	-2.701882	C	-2.915027	3.158410	-1.819757
H	4.050692	4.614166	-2.928459	C	-3.822312	4.216991	-1.941678
H	5.117935	5.592817	-0.902363	C	-4.417597	4.769402	-0.809450
H	4.550595	4.678151	1.341737	C	-4.096568	4.253497	0.451900
H	2.964786	2.782894	1.563711	C	-3.202303	3.194464	0.586696

Table A1.5 (Continued).

Atom	X	Y	Z
H	-2.970034	2.781881	1.565500
H	-4.555220	4.677515	1.341724
H	-5.118685	5.593190	-0.902931
H	-4.048273	4.615178	-2.927662
H	-2.399361	2.770271	-2.699120

Table A1.5 (Continued).

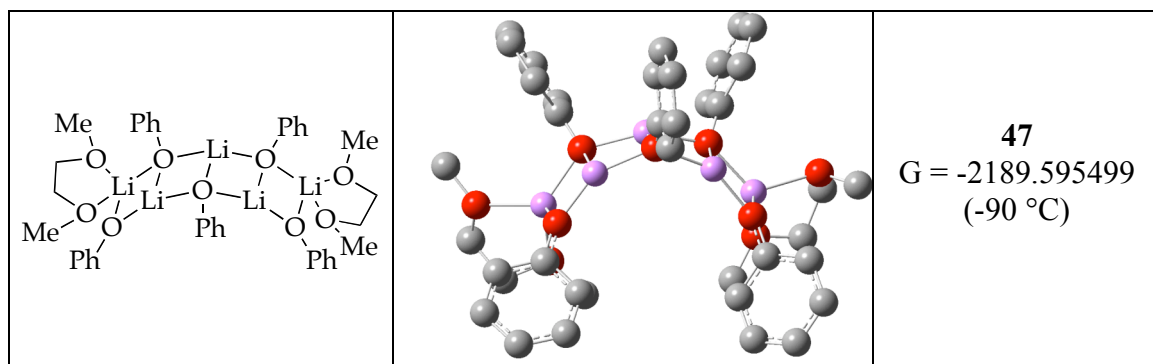
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Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.000653	1.556974	0.129381	H	2.400990	2.769737	-2.701882
O	-1.771208	1.557245	-0.460087	H	4.050692	4.614166	-2.928459
Li	-1.728224	-0.304600	0.410940	H	5.117935	5.592817	-0.902363
O	0.000738	-0.098846	1.138327	H	4.550595	4.678151	1.341737
Li	1.728544	-0.303623	0.407961	H	2.964786	2.782894	1.563711
O	1.769005	1.557665	-0.463503	C	0.001793	-0.395068	2.464451
Li	2.965986	0.557787	-1.528135	C	0.002425	-1.736321	2.896866
O	2.943323	-1.021245	-0.749065	C	0.003539	-2.041607	4.258947
C	3.514425	-2.228982	-0.898966	C	0.004042	-1.025535	5.217429
C	4.812491	-2.481059	-0.411404	C	0.003402	0.306412	4.797375
C	5.400995	-3.735807	-0.569680	C	0.002302	0.623261	3.438161
C	4.717070	-4.768704	-1.215212	H	0.001801	1.662796	3.114883
C	3.430062	-4.528035	-1.702007	H	0.003766	1.108665	5.531332
C	2.832624	-3.276875	-1.549479	H	0.004916	-1.267970	6.276043
H	1.830767	-3.088151	-1.928879	H	0.004030	-3.083329	4.569600
H	2.882882	-5.321514	-2.206264	H	0.002083	-2.527527	2.150388
H	5.178521	-5.744825	-1.335543	O	-2.943657	-1.022711	-0.745062
H	6.403433	-3.906475	-0.183261	Li	-2.968935	0.556873	-1.523176
H	5.342462	-1.677018	0.094643	C	-3.515032	-2.230153	-0.896316
C	2.589404	2.625748	-0.553808	C	-4.813142	-2.482483	-0.408996
C	3.198647	3.195060	0.585104	C	-5.401949	-3.736902	-0.568788
C	4.093315	4.253866	0.451334	C	-4.718305	-4.769164	-1.215621
C	4.416547	4.769193	-0.809704	C	-3.431242	-4.528247	-1.702158
C	3.823048	4.216426	-1.942682	C	-2.833493	-3.277425	-1.548118
C	2.915341	3.158084	-1.821790	H	-1.831589	-3.088445	-1.927257

Table A1.5 (Continued).

Atom	X	Y	Z
H	-2.884265	-5.321257	-2.207366
H	-5.180031	-5.745011	-1.337112
H	-6.404423	-3.907824	-0.182573
H	-5.342850	-1.678927	0.098090
C	-2.591285	2.625540	-0.551446
C	-2.915027	3.158410	-1.819757
C	-3.822312	4.216991	-1.941678
C	-4.417597	4.769402	-0.809450
C	-4.096568	4.253497	0.451900
C	-3.202303	3.194464	0.586696
H	-2.970034	2.781881	1.565500
H	-4.555220	4.677515	1.341724
H	-5.118685	5.593190	-0.902931
H	-4.048273	4.615178	-2.927662
H	-2.399361	2.770271	-2.699120

Table A1.5 (Continued).

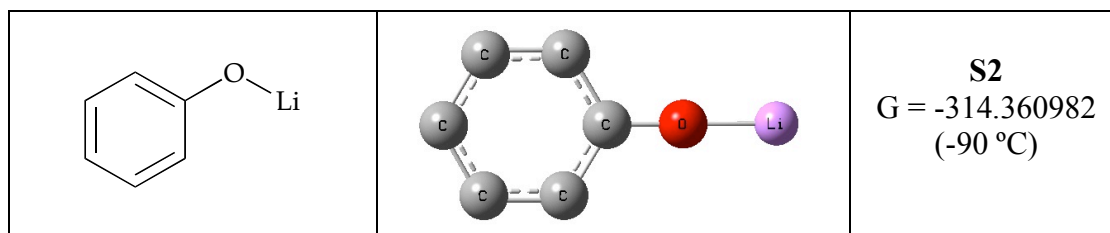


Atom	X	Y	Z	Atom	X	Y	Z
Li	1.717624	0.156932	1.276664	H	-4.776871	0.029252	-4.296978
O	-0.006416	-0.215072	1.959710	C	-2.552417	1.325266	-3.538392
Li	-0.014581	-1.494956	0.502300	H	-1.504990	1.220137	-3.250580
O	-1.828911	-1.313270	-0.042993	H	-2.640183	1.229288	-4.628917
Li	-1.694479	0.199333	1.219706	H	-2.920826	2.307929	-3.218212
O	-2.771302	1.336953	0.316456	C	-3.025814	2.643027	0.267815
Li	-3.063249	-0.072391	-0.855424	C	-2.205739	3.524944	-0.475334
C	-2.298674	-2.576954	-0.132137	C	-2.483004	4.890512	-0.536020
C	-2.190790	-3.300275	-1.339565	C	-3.582915	5.427869	0.137527
C	-2.671065	-4.607639	-1.434296	C	-4.397550	4.572174	0.883674
C	-3.268613	-5.229313	-0.335354	C	-4.128731	3.205342	0.951500
C	-3.378518	-4.523054	0.865343	H	-4.758274	2.546334	1.544830
C	-2.902562	-3.215825	0.971236	H	-5.251821	4.973520	1.425345
H	-2.997417	-2.666869	1.905566	H	-3.794714	6.492378	0.090600
H	-3.840560	-4.992048	1.731036	H	-1.827662	5.542190	-1.110696
H	-3.638806	-6.247695	-0.411622	H	-1.337693	3.112708	-0.985687
H	-2.572626	-5.144729	-2.375224	C	-0.043818	-0.253727	3.313033
H	-1.719201	-2.816917	-2.192355	C	-0.110846	0.938857	4.062754
O	-5.033959	-0.660654	-1.002790	C	-0.151463	0.899755	5.457383
C	-5.998950	0.162524	-0.344269	C	-0.125921	-0.319978	6.137946
H	-5.700032	0.209105	0.702993	C	-0.058153	-1.506089	5.403127
H	-6.016052	1.180944	-0.750831	C	-0.017230	-1.479711	4.008529
H	-6.996678	-0.288077	-0.425471	H	0.036505	-2.405955	3.440036
C	-5.273979	-0.871585	-2.393570	H	-0.036315	-2.464159	5.917385
H	-4.800207	-1.827735	-2.635676	H	-0.156930	-0.345857	7.223448
H	-6.350602	-0.948136	-2.597327	H	-0.201910	1.832765	6.013561
O	-3.264965	0.276159	-2.885914	H	-0.126222	1.888610	3.532779
C	-4.650038	0.239117	-3.224121	O	1.804077	-1.348756	-0.022453
H	-5.112702	1.213463	-3.006193	Li	2.978046	-0.072520	-0.902399

Table A1.5 (Continued).

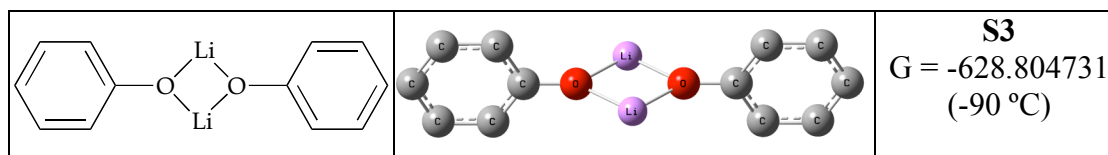
Atom	X	Y	Z
O	2.848561	1.248245	0.405153
C	3.341021	2.483872	0.427873
C	2.493475	3.615068	0.495719
C	3.018804	4.907222	0.499484
C	4.398208	5.121998	0.433045
C	5.248568	4.014699	0.369532
C	4.735472	2.717702	0.366527
H	5.399339	1.856476	0.336592
H	6.326395	4.160826	0.328441
H	4.802063	6.130655	0.438660
H	2.340022	5.755805	0.557393
H	1.418387	3.455105	0.549297
C	2.335859	-2.588378	-0.003895
C	3.065412	-3.058241	1.110130
C	3.612461	-4.342564	1.115886
C	3.451650	-5.192868	0.018830
C	2.729125	-4.740031	-1.088414
C	2.178414	-3.457873	-1.105199
H	1.615254	-3.104926	-1.966094
H	2.587848	-5.391323	-1.948104
H	3.875617	-6.192875	0.029553
H	4.167614	-4.679792	1.988271
H	3.194241	-2.400996	1.967721
O	2.726881	0.771765	-2.770275
C	4.053679	1.062306	-3.207675
H	4.050187	1.381516	-4.260665
H	4.479359	1.867922	-2.592516
C	1.854693	1.899929	-2.854003
H	1.745625	2.220290	-3.899333
H	0.886875	1.574742	-2.467286
H	2.225858	2.731229	-2.243370
O	4.783906	-0.620255	-1.700998
C	4.867424	-0.206810	-3.060132
H	5.913489	-0.010120	-3.338440
H	4.473643	-0.997933	-3.716181
C	5.548276	-1.792077	-1.419559
H	6.615084	-1.602542	-1.599300
H	5.385438	-2.034580	-0.369411
H	5.212887	-2.635187	-2.036492

Table A1.5 (Continued).



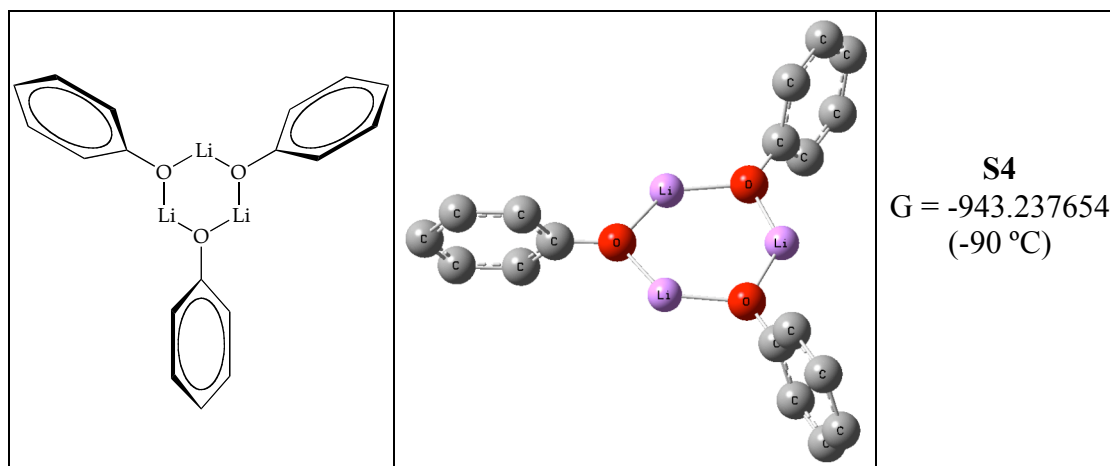
Atom	X	Y	Z	Atom	X	Y	Z
C	0.000137	-2.038685	0.000000	H	2.145002	0.619400	0.000000
C	-1.202935	-1.327374	0.000000	O	-0.000245	2.121447	0.000000
C	-1.208485	0.065889	0.000000	Li	-0.000416	3.743306	0.000000
C	0.000000	0.796987	0.000000	H	-2.145198	0.618957	0.000000
C	1.208602	0.065971	0.000000	H	-2.149816	-1.864023	0.000000
C	1.203173	-1.327236	0.000000	H	0.000151	-3.125338	0.000000
H	2.150113	-1.863799	0.000000				

Table A1.5 (Continued).



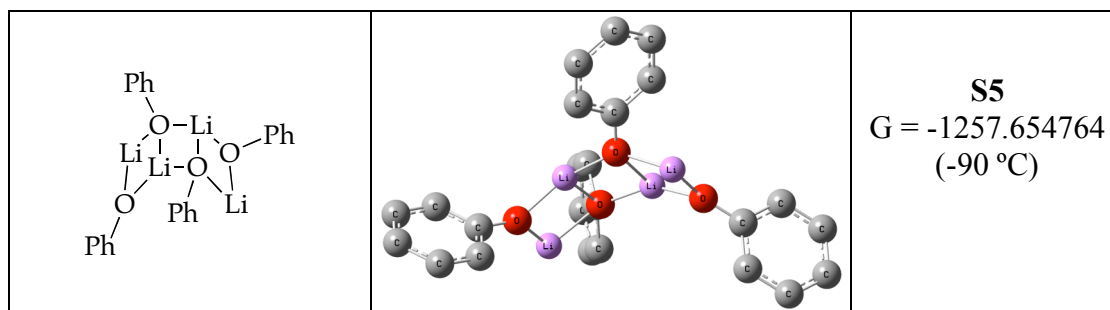
Atom	X	Y	Z	Atom	X	Y	Z
C	2.713146	0.000509	0.000435	C	4.833768	1.201606	-0.003630
C	3.435852	1.209164	0.002346	C	3.439119	1.209620	-0.001352
C	4.830537	1.204857	0.003476	H	2.887009	2.146919	-0.001753
C	5.540441	0.001723	0.001880	H	5.372221	2.146784	-0.005970
C	4.832447	1.202517	0.000898	H	6.626783	0.005519	-0.004626
C	3.437751	1.209021	0.002053	H	5.364091	2.152981	0.000871
H	2.884704	2.145773	0.004202	H	2.878994	2.143860	0.004929
H	5.369848	2.148295	0.002191	Li	0.000978	0.000689	1.169437
H	6.626779	0.002594	0.002781	C	2.713147	0.001881	0.001741
H	5.366470	2.151466	0.005659	C	3.434511	1.208559	0.002524
H	2.881265	2.145007	0.003576	C	4.829227	1.205765	0.000225
O	1.369205	0.001554	0.001536	C	5.540448	0.003442	-0.002857
Li	0.000795	0.004256	-1.164322	C	4.833768	1.201606	-0.003630
O	1.369236	0.004566	0.003817	C	3.439119	1.209620	-0.001352
Li	0.000978	0.000689	1.169437	H	2.887009	2.146919	-0.001753
C	2.713147	0.001881	0.001741	H	5.372221	2.146784	-0.005970
C	3.434511	1.208559	0.002524	H	6.626783	0.005519	-0.004626
C	4.829227	1.205765	0.000225	H	5.364091	2.152981	0.000871
C	5.540448	0.003442	-0.002857	H	2.878994	2.143860	0.004929

Table A1.5 (Continued).



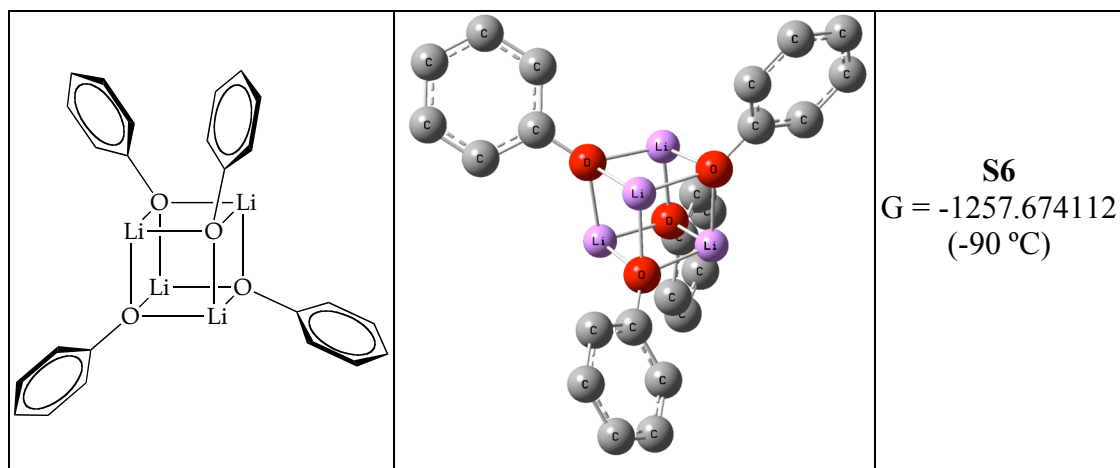
Atom	X	Y	Z	Atom	X	Y	Z
C	2.069417	-2.495842	0.017862	C	-5.983235	-1.018257	0.004698
C	2.418869	-3.169197	-1.169423	C	-5.285275	-0.943464	-1.202888
C	3.310709	-4.241647	-1.141474	C	-3.909988	-0.709375	-1.216986
C	3.875780	-4.667942	0.062716	H	-3.364301	-0.649606	-2.156194
C	3.535784	-4.005369	1.244339	H	-5.814197	-1.067955	-2.144993
C	2.643711	-2.932657	1.228016	H	-7.054020	-1.200472	0.011295
H	2.372608	-2.419180	2.148011	H	-5.814110	-0.911327	2.152234
H	3.966417	-4.325587	2.190274	H	-3.364252	-0.494477	2.133645
H	4.570300	-5.502921	0.079868	C	1.126315	3.039005	-0.034540
H	3.566246	-4.746298	-2.070351	C	1.607624	3.644876	-1.211907
H	1.982065	-2.831663	-2.106865	C	2.093883	4.952305	-1.190335
O	1.205011	-1.456935	-0.004029	C	2.111889	5.686874	-0.002368
Li	1.654226	0.280478	-0.026645	C	1.635945	5.094367	1.169513
O	0.655702	1.772306	-0.050969	C	1.149073	3.786855	1.159490
Li	-1.074472	1.293896	-0.045560	H	0.787238	3.320343	2.073368
O	-1.865682	-0.316009	-0.020829	H	1.644480	5.652400	2.102956
Li	-0.585361	-1.573845	-0.001484	H	2.490830	6.704747	0.009974
C	-3.198099	-0.543881	-0.012336	H	2.459522	5.399845	-2.111623
C	-3.909870	-0.620892	1.201018	H	1.583949	3.074199	-2.137805
C	-5.285232	-0.855515	1.203589				

Table A1.5 (Continued).



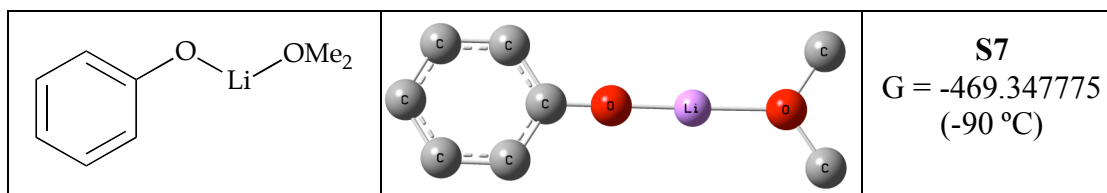
Atom	X	Y	Z	Atom	X	Y	Z
Li	1.235419	-0.039225	-0.341376	H	-3.067206	-0.474040	3.070992
O	-0.021377	-1.419237	-0.488498	O	-0.062453	1.485038	-0.415535
C	0.208946	-2.594839	-1.114897	Li	1.338291	2.189915	0.646873
C	1.401766	-3.319474	-0.899971	O	2.489934	0.852677	0.649136
C	1.594450	-4.557802	-1.507304	C	3.683347	0.512329	1.162390
C	0.608020	-5.117535	-2.327957	C	3.781563	-0.078604	2.438735
C	-0.576934	-4.415749	-2.541693	C	5.023128	-0.434157	2.965805
C	-0.780274	-3.165833	-1.946691	C	6.196387	-0.211906	2.241025
H	-1.686388	-2.597738	-2.154629	C	6.109579	0.374401	0.975883
H	-1.349369	-4.830658	-3.184374	C	4.873203	0.734005	0.439630
H	0.766359	-6.085341	-2.794221	H	4.804623	1.194209	-0.543590
H	2.522762	-5.095878	-1.332313	H	7.013441	0.555890	0.398438
H	2.161704	-2.898341	-0.245224	H	7.161492	-0.490205	2.654919
Li	-1.332043	0.118995	-0.350148	H	5.072478	-0.888718	3.952925
Li	-1.502374	-2.184017	0.399579	H	2.867167	-0.251154	3.002366
O	-2.636224	-0.834169	0.504556	C	-0.168689	2.669639	-1.055564
C	-3.825872	-0.546433	1.057318	C	0.041364	2.786416	-2.445797
C	-3.956027	-0.376784	2.450838	C	-0.003346	4.034105	-3.062698
C	-5.194405	-0.081762	3.020767	C	-0.247794	5.196088	-2.320961
C	-6.333013	0.052932	2.222951	C	-0.461020	5.094418	-0.947769
C	-6.214293	-0.112441	0.840801	C	-0.427178	3.845801	-0.316650
C	-4.980947	-0.409088	0.261316	H	-0.665434	3.757635	0.744227
H	-4.890011	-0.546427	-0.813983	H	-0.671481	5.983897	-0.359449
H	-7.091113	-0.012074	0.204867	H	-0.277871	6.163945	-2.812117
H	-7.295857	0.283202	2.670239	H	0.159960	4.102286	-4.135376
H	-5.268231	0.045096	4.098675	H	0.244275	1.886569	-3.021449

Table A1.5 (Continued).



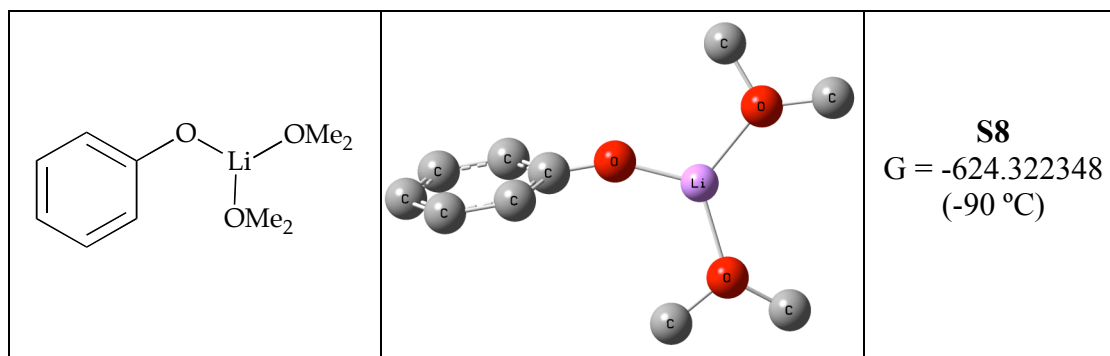
Atom	X	Y	Z	Atom	X	Y	Z
O	0.088214	1.491101	0.770560	H	-2.932011	-2.447042	-1.217086
Li	1.373229	0.127329	0.440394	H	-5.206008	-2.678587	-2.168751
O	0.290501	-1.362177	0.924284	H	-6.530747	-0.656534	-2.773193
Li	-0.167909	-1.334068	-0.943993	C	0.503313	-2.464637	1.674106
O	-1.679740	-0.164416	-0.786702	C	-0.571169	-3.151924	2.272697
Li	-1.073143	-0.016324	1.022406	C	-0.347450	-4.288065	3.050956
Li	-0.355293	1.188570	-1.078662	C	0.947491	-4.771203	3.250084
O	1.064461	-0.001989	-1.482919	C	2.019267	-4.101561	2.655221
C	2.258902	0.100391	-2.100888	C	1.804701	-2.965488	1.875281
C	2.932860	1.338141	-2.168333	H	2.643978	-2.452584	1.408175
C	4.180110	1.439285	-2.786900	H	3.033921	-4.466144	2.796801
C	4.787537	0.316411	-3.351814	H	1.118906	-5.655377	3.857016
C	4.128662	-0.914370	-3.289506	H	-1.194465	-4.798720	3.502908
C	2.882895	-1.026066	-2.673554	H	-1.584547	-2.785411	2.115070
H	2.373222	-1.986780	-2.630922	C	0.066606	2.640296	1.478916
H	4.587197	-1.798339	-3.726086	C	-1.142615	3.333342	1.691212
H	5.757210	0.398347	-3.833967	C	-1.166527	4.517817	2.428387
H	4.676384	2.405926	-2.828426	C	0.008479	5.043328	2.969561
H	2.460533	2.219383	-1.736879	C	1.212249	4.365877	2.761742
C	-2.926194	-0.290606	-1.288671	C	1.245494	3.181363	2.026640
C	-3.691394	0.843813	-1.624372	H	2.188085	2.660338	1.866722
C	-4.974345	0.709010	-2.155018	H	2.136882	4.761587	3.175146
C	-5.531860	-0.555019	-2.359210	H	-0.013040	5.965288	3.543138
C	-4.786203	-1.686358	-2.021308	H	-2.112666	5.032484	2.578330
C	-3.502449	-1.560402	-1.490364	H	-2.061033	2.930714	1.266382

Table A1.5 (Continued).



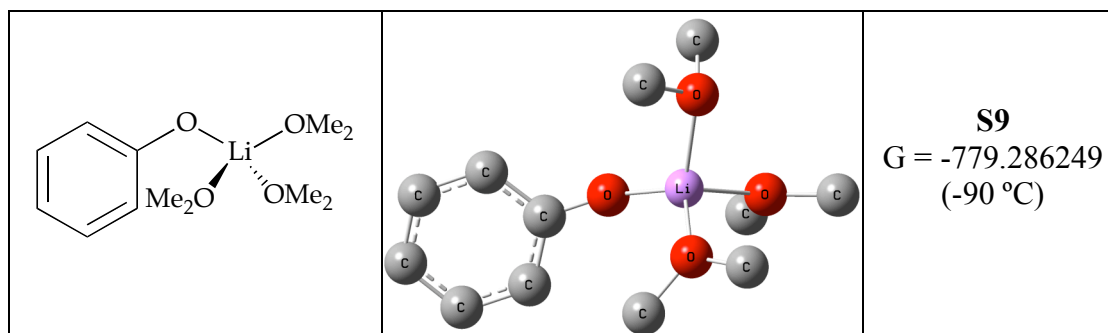
Atom	X	Y	Z	Atom	X	Y	Z
C	4.351507	1.196603	0.095597	H	-3.958030	-2.143218	0.089626
O	3.581022	-0.002253	-0.011255	H	-5.213485	0.009985	0.012596
Li	1.682009	-0.018204	-0.018163	H	-3.942248	2.153322	-0.076413
O	0.034879	-0.010253	-0.011751	H	-1.460458	2.139462	-0.087722
C	-1.283336	-0.005237	-0.005636	C	4.382918	-1.183275	-0.077852
C	-2.016337	1.204860	-0.048709	H	4.989554	-1.286687	0.830461
C	-3.409160	1.204585	-0.042190	H	5.039041	-1.151696	-0.956570
C	-4.126696	0.005752	0.007524	H	3.702280	-2.033281	-0.160858
C	-3.418014	-1.198595	0.050464	H	3.648636	2.031199	0.141252
C	-2.025180	-1.209604	0.044275	H	5.002007	1.313101	-0.780189
H	-1.476238	-2.148465	0.078162	H	4.961492	1.180414	1.007354

Table A1.5 (Continued).



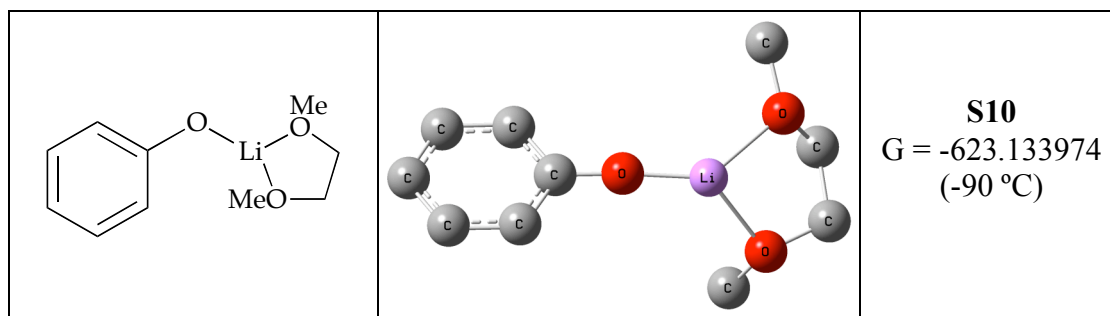
Atom	X	Y	Z	Atom	X	Y	Z
C	-2.036714	-2.716516	0.056135	C	4.409985	-0.074351	-0.000962
O	-2.676744	-1.432393	0.069995	C	3.666214	0.256348	1.135141
Li	-1.358918	-0.006364	0.012776	C	2.281291	0.100494	1.155595
O	-1.786714	1.886260	-0.067205	H	1.708430	0.343988	2.048870
C	-0.622547	2.719530	0.008805	H	4.172032	0.638288	2.020739
H	-0.451744	3.220631	-0.952857	H	5.489873	0.047348	-0.012530
H	0.219672	2.066349	0.239726	H	4.295899	-0.834035	-2.016946
H	-0.749083	3.473430	0.796912	H	1.830926	-1.115667	-1.987612
C	-2.962748	2.605313	-0.406501	C	-4.081578	-1.508358	0.249068
H	-3.786167	1.888363	-0.450502	H	-4.469594	-0.486729	0.254437
H	-2.855008	3.093268	-1.385072	H	-4.329723	-1.993390	1.203382
H	-3.187074	3.368289	0.351498	H	-4.551597	-2.070038	-0.570114
O	0.269833	-0.539376	0.038572	H	-0.968341	-2.516965	-0.047677
C	1.576679	-0.395502	0.027430	H	-2.407908	-3.313645	-0.787324
C	2.351632	-0.728124	-1.114208	H	-2.236074	-3.247600	0.996253
C	3.734658	-0.568621	-1.122235				

Table A1.5 (Continued).



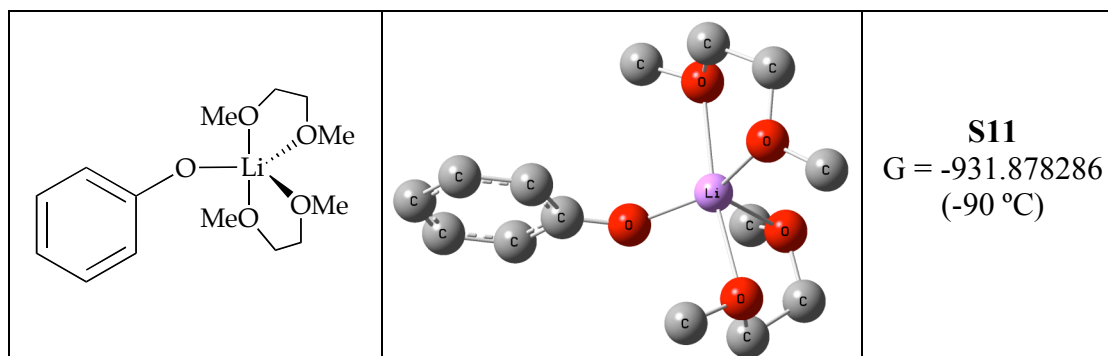
Atom	X	Y	Z	Atom	X	Y	Z
Li	1.055463	0.045891	-0.020149	H	4.001234	-1.097933	-2.353457
O	-0.604407	0.053448	-0.603313	H	4.044316	-0.757084	-0.600365
C	-1.902492	0.002595	-0.422181	O	1.300760	-0.640954	1.853878
C	-2.590512	-1.234802	-0.284417	C	2.504820	-0.835568	2.576737
C	-3.968877	-1.286000	-0.086393	H	2.401185	-0.487008	3.614393
C	-4.730399	-0.115781	-0.019546	H	2.794198	-1.896514	2.588066
C	-4.077114	1.113482	-0.159581	H	3.281695	-0.250848	2.078174
C	-2.700492	1.177337	-0.357438	C	0.186039	-1.328181	2.424850
H	-2.203715	2.138503	-0.478482	H	-0.011171	-0.958067	3.440470
H	-4.651735	2.037738	-0.116287	H	-0.671633	-1.132073	1.780823
H	-5.805311	-0.159584	0.134334	H	0.381340	-2.409052	2.467839
H	-4.456565	-2.254810	0.013601	O	1.937402	1.875556	0.056900
H	-2.006823	-2.151703	-0.351012	C	1.907951	2.459843	-1.245415
O	2.174005	-0.968342	-1.364326	H	2.414000	3.435167	-1.240411
C	1.396254	-1.635970	-2.361633	H	2.435403	1.774559	-1.911106
H	1.462858	-2.725682	-2.233907	H	0.872940	2.576821	-1.590573
H	0.370163	-1.296617	-2.209778	C	1.266138	2.688759	1.018782
H	1.753845	-1.368739	-3.365993	H	0.212497	2.825331	0.743408
C	3.542266	-1.332697	-1.381935	H	1.323868	2.163211	1.973364
H	3.669754	-2.406840	-1.182859	H	1.757696	3.667774	1.104111

Table A1.5 (Continued).



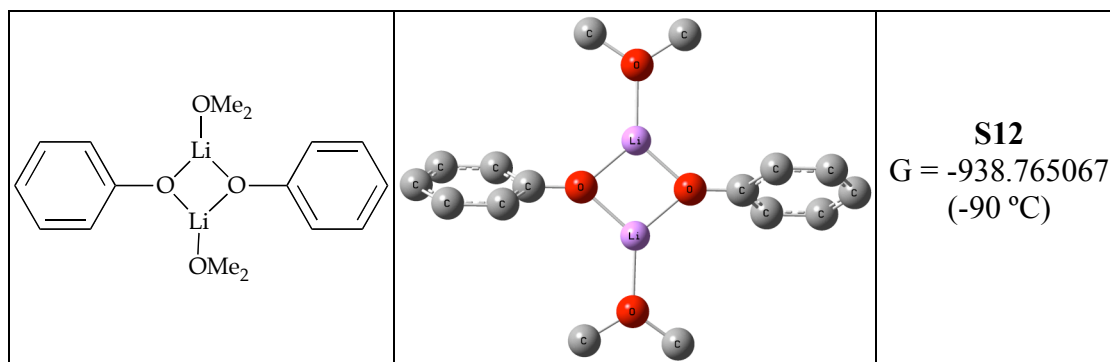
Atom	X	Y	Z	Atom	X	Y	Z
C	-3.538729	0.507852	0.383835	O	-2.332468	-1.509627	-0.206336
O	-2.663246	1.162153	-0.534217	C	-3.637752	-0.942627	-0.068236
Li	-1.092465	-0.058173	-0.788494	H	-4.100364	-0.990710	-1.059067
O	0.541695	0.057311	-0.444543	H	-4.248648	-1.526950	0.631330
C	1.838410	0.059337	-0.227766	C	-1.835643	-2.190672	0.954448
C	2.444620	1.007805	0.634262	H	-1.890027	-1.555483	1.847537
C	3.817852	1.001612	0.866947	H	-0.790009	-2.422685	0.749546
C	4.646547	0.056455	0.254761	H	-2.406058	-3.112520	1.120955
C	4.067618	-0.886636	-0.600283	C	-2.433826	2.539636	-0.228580
C	2.695801	-0.889624	-0.840097	H	-2.003635	2.648813	0.775072
H	2.249965	-1.623500	-1.508838	H	-1.724408	2.912887	-0.968394
H	4.695041	-1.630723	-1.088724	H	-3.371215	3.106588	-0.293558
H	5.717732	0.055306	0.438646	H	-4.531770	0.980749	0.375022
H	4.248264	1.745586	1.535748	H	-3.128804	0.583221	1.402634
H	1.804099	1.746407	1.112607				

Table A1.5 (Continued).



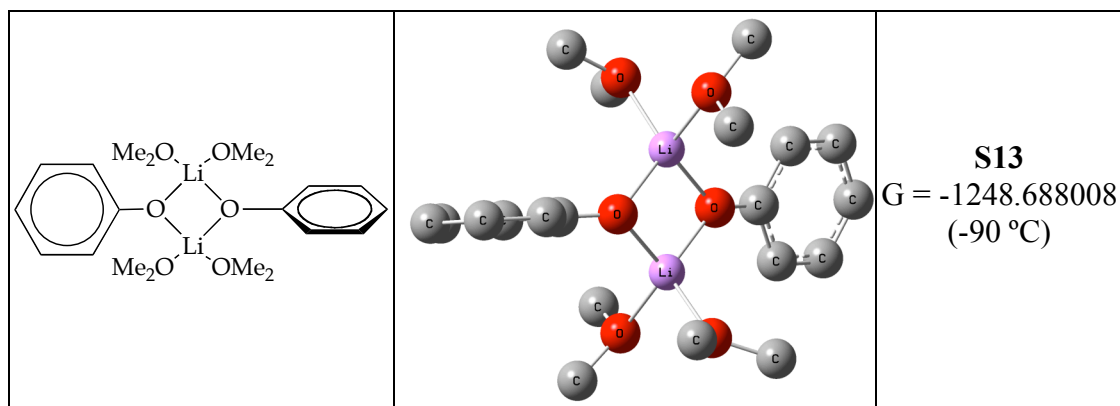
Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.893184	0.064374	0.090176	H	-0.944364	3.995166	0.597266
O	0.784302	-0.592885	0.242668	H	-0.099419	2.997474	-0.617693
C	2.050183	-0.376311	-0.011097	C	0.643332	2.210101	1.766774
C	2.478565	0.516874	-1.034935	H	0.786356	1.380583	2.458550
C	3.829651	0.743682	-1.292098	H	0.637916	3.161601	2.317804
C	4.822013	0.097386	-0.549841	H	1.459581	2.201154	1.035774
C	4.427405	-0.788092	0.459750	O	-1.540155	-1.710317	-1.233024
C	3.081851	-1.022169	0.726691	C	-1.491976	-2.702284	-0.211583
H	2.786378	-1.714876	1.512669	C	-2.457906	-2.268362	0.877564
H	5.183820	-1.304047	1.049669	O	-2.070762	-1.032402	1.485877
H	5.874467	0.275473	-0.753677	C	-1.233854	-1.185704	2.639207
H	4.111465	1.434039	-2.086257	H	-0.237438	-1.539679	2.355925
H	1.713839	1.018705	-1.627525	H	-1.704711	-1.866599	3.361198
O	-0.618005	2.006240	1.126157	H	-1.147291	-0.193162	3.085696
C	-0.893252	2.991687	0.145150	H	-2.549223	-3.053955	1.640227
C	-2.226272	2.652466	-0.485378	H	-3.447166	-2.097012	0.439796
O	-2.131860	1.342757	-1.034034	H	-0.467495	-2.775223	0.175051
C	-3.342845	0.910007	-1.645271	H	-1.801229	-3.681621	-0.613074
H	-3.179800	-0.118636	-1.964818	C	-0.583592	-1.945954	-2.266183
H	-4.175153	0.945033	-0.927645	H	0.431546	-1.896839	-1.860662
H	-3.588285	1.543486	-2.509240	H	-0.762933	-2.920878	-2.742548
H	-3.025359	2.681971	0.270803	H	-0.718913	-1.154868	-3.007682
H	-2.465017	3.382483	-1.273795				

Table A1.5 (Continued).



Atom	X	Y	Z	Atom	X	Y	Z
C	1.135185	-3.906757	-0.162174	C	-1.166091	3.899007	-0.141923
O	-0.034913	-3.110241	0.012836	H	-2.005121	3.203186	-0.207688
Li	0.000189	-1.199756	0.099909	H	-1.273664	4.524158	0.754643
O	1.383594	-0.004592	0.061397	H	-1.148361	4.541469	-1.032529
Li	0.013563	1.206414	0.007050	C	2.712800	-0.013818	0.043961
O	-1.371116	0.011779	0.061393	C	3.429504	-0.528898	-1.062014
C	-2.699614	0.013209	0.044743	C	4.823934	-0.537121	-1.074503
C	-3.420241	0.517418	-1.064125	C	5.553102	-0.034714	0.006633
C	-4.814619	0.518090	-1.075686	C	4.859464	0.478813	1.105994
C	-5.540504	0.017327	0.008488	C	3.465356	0.491532	1.129934
C	-4.843327	-0.485809	1.110423	H	2.927030	0.875461	1.994168
C	-3.449141	-0.489555	1.134143	H	5.410239	0.870934	1.958807
H	-2.908756	-0.863671	2.001469	H	6.639439	-0.042871	-0.007292
H	-5.391312	-0.876269	1.965789	H	5.346518	-0.936881	-1.941456
H	-6.626861	0.019046	-0.005019	H	2.863437	-0.903610	-1.912546
H	-5.339793	0.909890	-1.944698	C	-1.247650	-3.859604	-0.013504
H	-2.857132	0.889632	-1.917871	H	-2.067020	-3.152479	0.130924
O	0.024175	3.117148	-0.066705	H	-1.364158	-4.367520	-0.980183
C	1.217398	3.893866	0.010779	H	-1.256694	-4.605665	0.792461
H	1.198285	4.540600	0.898194	H	1.094539	-4.443273	-1.119926
H	2.052757	3.194309	0.084626	H	1.990871	-3.228446	-0.158625
H	1.332806	4.514053	-0.888140	H	1.234426	-4.632695	0.655641

Table A1.5 (Continued).

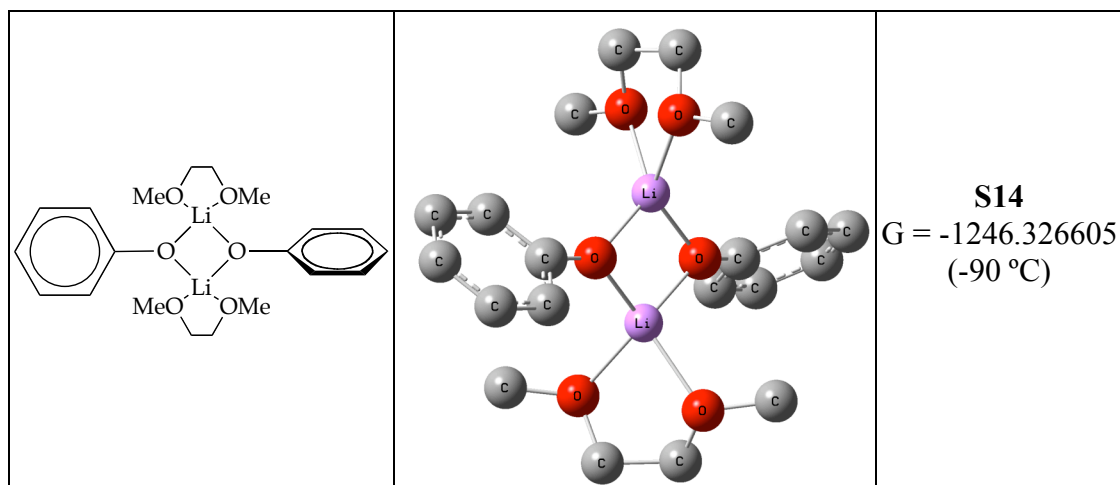


Atom	X	Y	Z	Atom	X	Y	Z
C	0.712005	2.348694	-2.488717	H	-0.461989	-1.663872	-3.114447
O	0.052675	2.673072	-1.268433	H	0.711332	-3.014334	-3.168872
Li	0.080046	1.282401	0.199056	H	1.172849	-1.459897	-2.408000
O	1.421497	-0.029965	0.050047	C	-1.175158	-3.502813	-1.353063
Li	0.006549	-1.249657	0.220751	H	-2.058337	-3.016962	-1.788696
O	-1.353603	0.055344	0.364053	H	-1.393482	-3.806125	-0.327580
C	-2.626378	0.067943	0.003651	H	-0.911815	-4.389085	-1.947608
C	-3.667535	0.202271	0.957272	C	2.725180	-0.084700	-0.154282
C	-5.007994	0.209199	0.573851	C	3.538030	1.077545	-0.107292
C	-5.372992	0.084694	-0.769537	C	4.912328	1.014122	-0.329757
C	-4.363633	-0.046098	-1.727643	C	5.541185	-0.202736	-0.608522
C	-3.019803	-0.054988	-1.355091	C	4.759828	-1.360451	-0.661316
H	-2.238138	-0.154703	-2.105933	C	3.384528	-1.308647	-0.441680
H	-4.625560	-0.141738	-2.780087	H	2.786054	-2.216461	-0.494713
H	-6.418970	0.091086	-1.063174	H	5.227381	-2.319297	-0.878787
H	-5.778351	0.315458	1.335566	H	6.612979	-0.247500	-0.780547
H	-3.393900	0.307998	2.005004	H	5.501093	1.928702	-0.282643
O	-0.072037	-2.505366	1.810642	H	3.061761	2.030462	0.115601
C	1.121202	-2.981043	2.422053	C	-1.196404	3.330441	-1.472101
H	0.987253	-4.008607	2.789198	H	-1.598612	3.560241	-0.483706
H	1.905711	-2.958445	1.664219	H	-1.052142	4.261788	-2.037571
H	1.414120	-2.334713	3.261281	H	-1.900699	2.679027	-2.005217
C	-1.161479	-2.412678	2.720594	H	0.926785	3.261255	-3.062503
H	-2.001669	-1.983043	2.173955	H	1.646053	1.850213	-2.224534
H	-1.429130	-3.406676	3.106869	H	0.093768	1.677842	-3.101827
H	-0.908223	-1.758090	3.566967	O	0.066508	2.559243	1.772124
O	-0.077860	-2.598371	-1.289081	C	-0.312044	1.952116	3.002671
C	0.354783	-2.162190	-2.573127	H	-1.000288	1.146099	2.744934

Table A1.5 (Continued).

Atom	X	Y	Z
H	-0.809377	2.681847	3.657407
H	0.566005	1.541427	3.521714
C	1.022167	3.597698	1.935839
H	1.234758	3.992728	0.940736
H	0.619767	4.399727	2.571109
H	1.948883	3.213478	2.384846

Table A1.5 (Continued).

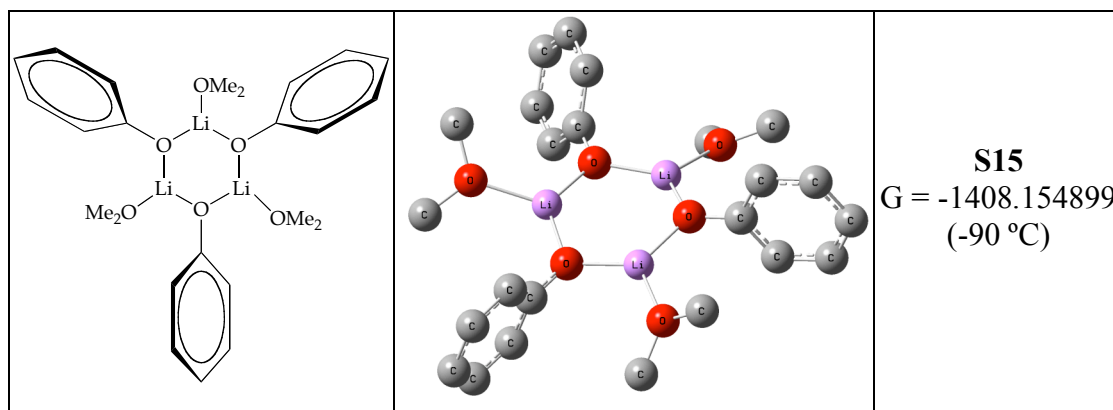


Atom	X	Y	Z	Atom	X	Y	Z
Li	0.006243	-1.242034	0.194769	H	-6.880171	-0.266530	-0.171263
O	-0.262288	-2.783350	-1.143046	H	-5.388604	1.226842	-1.694250
C	-0.129667	-4.032806	-0.476716	H	-2.890605	1.342308	-1.580848
C	0.958394	-3.876735	0.565856	Li	-0.047593	1.281600	0.159552
O	0.559213	-2.824066	1.437518	O	1.347151	0.055556	0.281737
C	1.527798	-2.529811	2.444334	C	2.653889	0.063483	0.074390
H	1.691905	-3.407399	3.084648	C	3.231027	-0.577159	-1.052134
H	2.475831	-2.211072	1.994986	C	4.609246	-0.577073	-1.270129
H	1.121019	-1.712136	3.040748	C	5.441203	0.065586	-0.361813
H	1.081136	-4.817086	1.124034	C	4.924282	0.706302	0.757724
H	1.916455	-3.623484	0.087685	C	3.545909	0.702397	0.972122
H	-1.081155	-4.303172	0.005572	H	3.128871	1.193607	1.848233
H	0.139627	-4.827141	-1.189106	H	5.601239	1.198997	1.450035
C	-1.369904	-2.730126	-2.040891	H	6.786120	0.067497	-0.571768
H	-2.310890	-2.922542	-1.510224	H	5.043215	-1.067569	-2.137039
H	-1.243334	-3.460461	-2.851697	H	2.567029	-1.069735	-1.759373
H	-1.394061	-1.719623	-2.449207	O	0.427216	2.817139	-1.127871
O	-1.386718	-0.017096	0.095462	C	-0.286189	3.988018	-0.754605
C	-2.707322	-0.069493	0.039121	C	-0.175008	4.111929	0.753115
C	-3.442153	0.698609	-0.898713	O	-0.637810	2.888982	1.309303
C	-4.833711	0.636182	-0.970658	C	-0.636040	2.860444	2.731002
C	-5.522171	-0.201612	-0.102014	H	-1.298141	3.637954	3.135663
C	-4.848128	-0.974539	0.835511	H	-1.009969	1.877803	3.022934
C	-3.456459	-0.906630	0.904173	H	0.378739	3.004807	3.127919
H	-2.918577	-1.496391	1.643382	H	-0.786997	4.955372	1.106268
H	-5.414625	-1.617105	1.503745	H	0.870984	4.288337	1.046632

Table A1.5 (Continued).

Atom	X	Y	Z
H	-1.340758	3.901200	-1.057672
H	0.146567	4.877840	-1.235666
C	0.501494	2.598224	-2.531819
H	-0.500551	2.474648	-2.966333
H	1.081158	1.684394	-2.671067
H	1.011951	3.434960	-3.027632

Table A1.5 (Continued).

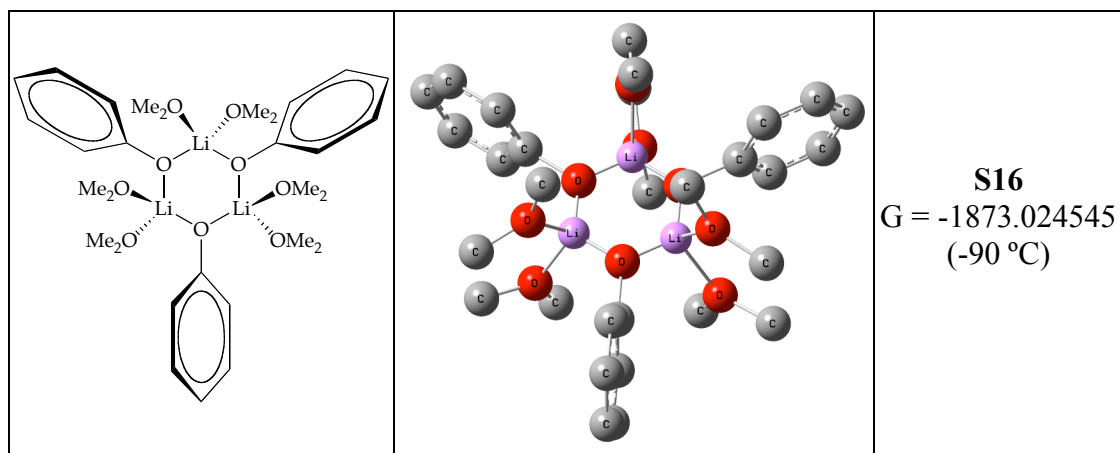


Atom	X	Y	Z	Atom	X	Y	Z
C	-3.757886	2.899576	-0.248735	C	2.860842	-1.434569	-0.235834
O	-3.295118	1.621730	-0.679487	C	3.692968	-1.581188	0.899038
Li	-1.597124	0.783585	-0.124085	C	4.937155	-2.203610	0.802716
O	-0.123660	1.853349	0.151508	C	5.397075	-2.703090	-0.419689
Li	1.491670	0.990841	-0.035007	C	4.586517	-2.568346	-1.549901
O	1.670435	-0.837822	-0.154004	C	3.339808	-1.945737	-1.465677
Li	0.113257	-1.774394	0.145378	H	2.710186	-1.837712	-2.346451
O	-1.576152	-1.053595	0.001706	H	4.926996	-2.950652	-2.510167
C	-2.684602	-1.794954	-0.031971	H	6.366795	-3.187900	-0.489252
C	-3.635229	-1.743322	1.014932	H	5.553951	-2.301290	1.693963
C	-4.795247	-2.517211	0.973023	H	3.334322	-1.197656	1.851818
C	-5.049835	-3.369309	-0.105110	O	3.126129	2.092249	-0.112473
C	-4.119691	-3.433594	-1.146570	C	3.326772	3.262421	0.677031
C	-2.957842	-2.662084	-1.116513	H	2.399615	3.456756	1.217579
H	-2.238629	-2.708594	-1.931765	H	4.152472	3.108177	1.385712
H	-4.300856	-4.090116	-1.995314	H	3.554198	4.125176	0.037185
H	-5.954009	-3.970928	-0.133050	C	4.265193	1.765849	-0.905311
H	-5.506671	-2.454689	1.794162	H	4.036872	0.845859	-1.444671
H	-3.436717	-1.084661	1.858040	H	5.143814	1.596530	-0.269275
O	0.221930	-3.639802	0.784373	H	4.480200	2.576388	-1.615530
C	-0.685245	-4.150060	1.758686	C	-0.219435	3.180316	0.253462
H	-1.131243	-5.091988	1.413341	C	-0.119169	4.017888	-0.882580
H	-0.166470	-4.322657	2.712230	C	-0.219442	5.403777	-0.765333
H	-1.475735	-3.410160	1.889374	C	-0.424075	6.005775	0.480120
C	1.268920	-4.558252	0.478796	C	-0.526618	5.192938	1.612006
H	0.850945	-5.489184	0.071403	C	-0.426246	3.804343	1.506931
H	1.857564	-4.787674	1.377029	H	-0.503954	3.171911	2.388896
H	1.915494	-4.084462	-0.260539	H	-0.685881	5.642780	2.590016

Table A1.5 (Continued).

Atom	X	Y	Z
H	-0.502153	7.085938	0.566091
H	-0.138367	6.020709	-1.658134
H	0.036184	3.550937	-1.852714
C	-4.172299	1.011680	-1.623311
H	-5.175702	0.889601	-1.194964
H	-3.766493	0.027257	-1.859096
H	-4.237945	1.622358	-2.534757
H	-4.734973	2.804205	0.244994
H	-3.022077	3.295632	0.452012
H	-3.847996	3.585713	-1.101234

Table A1.5 (Continued).

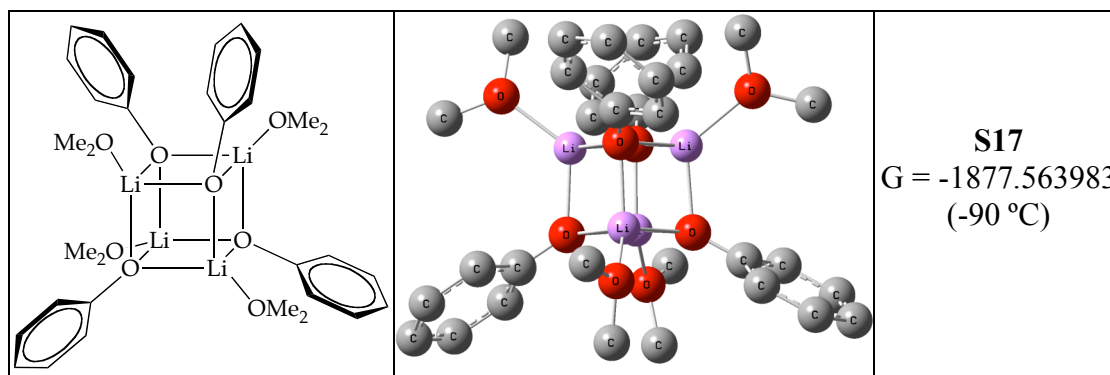


Atom	X	Y	Z	Atom	X	Y	Z
Li	-3.018404	1.912134	-0.001678	C	-5.953374	0.705847	-1.209607
Li	-0.925925	0.703703	0.000000	C	-7.348989	0.703398	1.206322
Li	-3.018623	-0.504047	0.000000	H	-5.404546	0.701421	2.159293
C	-0.853911	-1.837983	0.001841	C	-7.348199	0.706405	-1.209858
C	-0.505715	-2.440833	1.210375	H	-5.402949	0.707226	-2.161619
C	-0.504575	-2.443442	-1.205883	C	-8.046085	0.705576	-0.001816
C	0.190762	-3.649711	1.211942	H	-7.898973	0.702410	2.158508
H	-0.781192	-1.964126	2.162270	H	-7.898096	0.707707	-2.162268
C	0.192150	-3.651792	-1.204238	H	-9.145689	0.706214	-0.002259
H	-0.779172	-1.967900	-2.158643	O	-1.623579	1.912212	-0.001199
C	0.539514	-4.255192	0.004750	O	-3.716005	0.703928	-0.000682
H	0.464800	-4.125067	2.164876	O	-1.623463	-0.504047	0.000000
H	0.467619	-4.129211	-2.155901	C	1.768816	0.704332	1.479852
H	1.088603	-5.207888	0.005802	C	1.771354	0.702866	-1.475220
C	-0.853075	3.245600	-0.001281	C	-0.397071	0.701984	-3.028516
C	-0.501975	3.848365	-1.209016	C	-0.402275	0.704990	3.029420
C	-0.505783	3.850647	1.207239	H	0.374056	0.670780	-3.769656
C	0.195364	5.056748	-1.208992	H	-1.027799	-0.155928	-3.133717
H	-0.775840	3.371984	-2.161540	H	-0.979238	1.590547	-3.156721
C	0.191804	5.058500	1.207187	H	-0.590764	1.712935	3.335065
H	-0.782669	3.375171	2.159370	H	-1.324064	0.162365	3.001794
C	0.542074	5.661817	-0.001005	H	0.264560	0.240084	3.725187
H	0.471692	5.532037	-2.161297	H	2.172326	-0.169084	1.948065
H	0.465663	5.535594	2.159477	H	2.172314	1.578218	1.947199
H	1.091842	6.614121	-0.000802	H	2.175668	-0.171013	-1.941872
C	-5.256005	0.704184	-0.000934	H	2.175656	1.576288	-1.942739
C	-5.953829	0.702361	1.206650	O	0.238743	0.702780	-1.625897

Table A1.5 (Continued).

Atom	X	Y	Z
O	0.235948	0.704395	1.627896
O	-3.568283	-1.456924	-1.536879
O	-3.568283	-1.455188	1.537954
C	-4.430106	-2.530484	-1.150056
C	-4.450174	-2.513651	1.154777
H	-4.216925	-3.529275	-1.469225
H	-5.018756	-2.374940	-2.029941
H	-4.091820	-3.438994	1.555058
H	-5.430608	-2.316354	1.535202
C	-3.181949	-1.151456	-2.879390
C	-3.164563	-1.161660	2.878010
H	-2.394700	-0.426882	-2.867887
H	-4.022271	-0.756702	-3.411299
H	-2.839800	-2.042216	-3.363518
H	-2.152904	-1.478453	3.023223
H	-3.802259	-1.678960	3.564046
H	-3.236443	-0.107935	3.049462
O	-3.568595	2.865717	1.534573
O	-3.567539	2.862573	-1.540254
C	-4.249413	4.056093	-1.145975
C	-4.247663	4.059876	1.137395
H	-3.885897	5.013682	1.460318
H	-4.864946	3.998850	2.009254
H	-3.730757	4.907856	-1.533785
H	-5.247545	4.040437	-1.531186
C	-3.340934	2.456232	2.885644
C	-3.336755	2.451579	-2.890337
H	-2.323420	2.664759	-3.159793
H	-3.998451	2.982094	-3.542727
H	-3.515710	1.400356	-2.978692
H	-2.753115	1.562189	2.893129
H	-4.279342	2.270118	3.364865
H	-2.819998	3.229991	3.409880
H	2.027606	0.703383	-0.436358
H	2.026852	0.703818	0.441432
H	-4.280150	4.113041	-0.077934
H	-4.487971	-2.577604	0.087359
H	-5.288170	-2.335013	-0.541437
H	-5.117554	3.999567	0.517272

Table A1.5 (Continued).

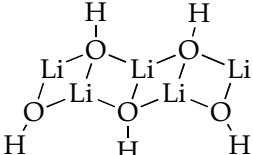
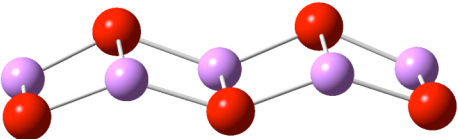


Atom	X	Y	Z	Atom	X	Y	Z
O	0.735744	0.150809	1.573617	H	4.344057	0.687785	-1.240599
Li	-0.017001	-1.448312	0.740469	H	5.157250	0.150038	-0.735138
O	-1.695349	-0.581158	0.196583	C	3.849996	0.017080	-1.945639
Li	-0.745702	-0.163833	-1.465126	H	4.759334	1.552106	-1.776617
O	-0.024207	1.540155	-0.840074	H	3.887956	1.985545	0.698766
Li	-0.849327	1.053843	0.880420	H	4.692678	1.493015	1.258957
O	-1.796917	2.475885	1.877358	C	4.271105	2.906038	0.237750
C	-1.246558	3.792034	1.919375	C	3.072861	2.224806	1.382987
H	-1.459989	4.263700	2.887901	C	-0.086855	2.720876	-1.452231
H	-0.166947	3.695068	1.792759	C	1.090128	3.423597	-1.797994
H	-1.651272	4.407918	1.107140	C	0.996948	4.653385	-2.432424
C	-3.209780	2.463345	2.076127	C	-0.215079	5.251637	-2.760649
H	-3.535103	1.422875	2.026161	H	-1.379983	4.556418	-2.424567
H	-3.459625	2.880874	3.060853	H	-1.329320	3.317515	-1.784561
H	-3.717343	3.047192	1.296464	H	-2.245264	2.790086	-1.528694
Li	1.498159	0.474023	-0.207360	O	-2.346781	4.990880	-2.668129
O	0.846870	-1.204713	-0.996767	C	-0.233568	6.214964	-3.257430
C	1.614960	-2.001632	-1.737338	H	2.147226	5.299751	-2.746138
C	2.162888	-3.189951	-1.201027	H	2.061367	2.998906	-1.566874
C	2.956013	-4.002237	-1.998333	H	-1.571199	-0.448846	-3.240446
C	3.258522	-3.708716	-3.323933	C	-1.417477	0.467617	-4.322966
C	2.725881	-2.530169	-3.852921	H	-0.554558	0.194142	-4.945538
C	1.921701	-1.687243	-3.085250	H	-2.322157	0.476781	-4.945658
H	1.516442	-0.772134	-3.510415	H	-1.262383	1.457089	-3.889555
H	2.944229	-2.264714	-4.884759	C	-1.794704	-1.788371	-3.678772
H	3.884163	-4.377859	-3.903772	C	-1.962875	-2.394304	-2.786582
O	3.459032	-5.137382	-1.454012	C	-2.684255	-1.836052	-4.320844
C	1.964006	-3.465274	-0.170206	C	-0.921824	-2.169839	-4.223165
H	3.361561	1.111041	-0.297515	C	-2.942473	-0.980349	0.438134

Table A1.5 (Continued).

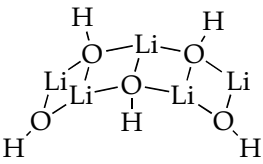
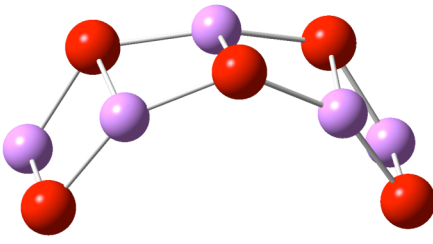
Atom	X	Y	Z
C	-3.915794	-0.990536	-0.587601
H	-5.205791	-1.416412	-0.307075
H	-5.612124	-1.838804	0.954341
H	-4.654677	-1.818908	1.972062
O	-3.346129	-1.399496	1.730835
C	-2.613468	-1.382574	2.534001
H	-4.937163	-2.135226	2.973508
H	-6.633425	-2.162217	1.120588
H	-6.112054	-1.418770	-1.315682
C	-3.655156	-0.659195	-1.587531
H	-0.087743	-3.230405	1.587431
H	-0.831078	-4.245944	0.914118
H	-1.887836	-4.213016	1.207939
C	-0.739019	-4.053244	-0.156392
C	-0.413555	-5.236193	1.139665
C	-0.063667	-3.411628	3.002536
C	0.388471	-4.380480	3.253585
C	0.544499	-2.607314	3.419761
C	-1.079476	-3.368106	3.417819
H	1.352599	0.184225	2.754704
H	0.861372	0.987474	3.808956
H	1.526453	1.004317	5.026471
F	2.673442	0.259171	5.278606
F	3.156961	-0.539318	4.238279
F	2.517961	-0.584212	2.999185
F	2.906605	-1.206955	2.197152
H	4.050545	-1.137933	4.398911
H	3.155619	0.308598	6.248352
H	1.029653	1.787067	6.015872
H	-0.037432	1.579090	3.668091

Table A1.5 (Continued).

		<p>S18 G = -417.175865 (-90 °C)</p>
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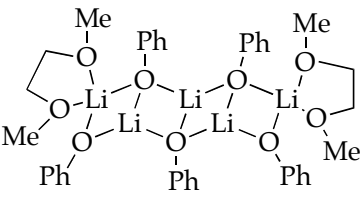
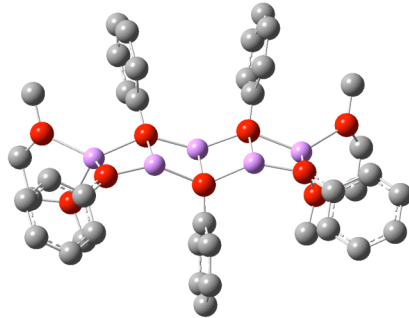
Atom	X	Y	Z
O	1.736811	1.329447	0.042905
Li	-0.000032	0.792012	-0.411985
O	-0.000060	-1.060908	0.076784
Li	1.766318	-0.652129	0.514006
O	3.479635	-0.916966	-0.035349
Li	3.380869	0.758009	-0.488110
H	3.977151	-1.713672	-0.242117
Li	-1.766408	-0.652347	0.514272
O	-1.736709	1.329533	0.042958
Li	-3.380578	0.757988	-0.488474
O	-3.479686	-0.916889	-0.035345
H	-3.977312	-1.713512	-0.242180
H	-1.698768	2.078380	0.653734
H	0.000081	-1.854186	-0.477399
H	1.698419	2.078655	0.653207

Table A1.5 (Continued).

		<p>S19 $G = -417.173551$ (-90 °C)</p>
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Atom	X	Y	Z
O	1.798560	-1.321300	-0.329324
Li	0.000106	-1.305359	0.203534
O	0.000041	0.115904	1.534593
Li	1.663005	0.442922	0.758107
O	2.741305	1.362086	-0.374109
Li	2.763191	-0.117660	-1.287542
H	2.888212	2.306443	-0.483625
Li	-1.662780	0.443058	0.758015
O	-1.798250	-1.321423	-0.329517
Li	-2.763344	-0.117880	-1.287384
O	-2.741716	1.361833	-0.373908
H	-2.888638	2.306172	-0.483588
H	-2.269470	-2.094631	0.010934
H	0.000073	-0.035459	2.489222
H	2.269776	-2.094567	0.010990

Table A1.5 (Continued).

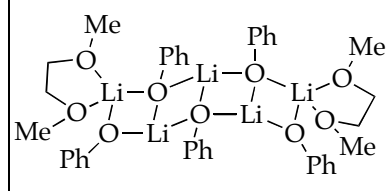
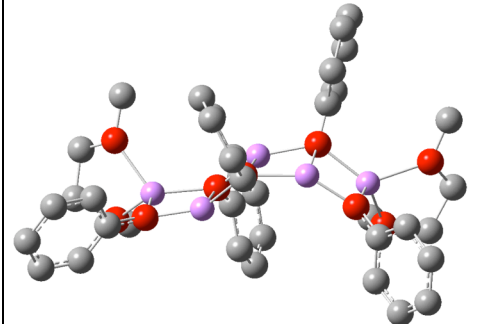
		<p>S20 G = -2189.592569 (-90 °C)</p>
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Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.016066	0.745896	0.390569	H	5.684857	1.995611	2.443645
O	-1.796734	1.197841	-0.001729	C	5.629962	2.857525	-0.086052
Li	-1.757762	-0.553401	-0.904184	H	6.697166	2.966467	-0.321510
O	-0.010667	-1.053992	-0.340113	H	5.324431	3.634368	0.625148
Li	1.730179	-0.522626	-0.904651	H	5.035743	2.956596	-0.994333
O	1.788058	1.181109	0.085890	C	2.007018	2.497210	-0.122515
Li	3.651571	0.468399	0.332463	C	2.147461	3.383649	0.966769
O	3.475753	-0.913282	-0.904437	C	2.385621	4.742532	0.756288
C	4.363037	-1.844181	-1.249540	C	2.494056	5.255285	-0.538938
C	5.608360	-1.489616	-1.819890	C	2.354162	4.386988	-1.624910
C	6.543973	-2.463610	-2.167681	C	2.116891	3.026544	-1.425505
C	6.276994	-3.820143	-1.962516	H	2.006614	2.353888	-2.273093
C	5.048991	-4.186100	-1.405061	H	2.426169	4.770910	-2.639928
C	4.105479	-3.221359	-1.051695	H	2.673693	6.314443	-0.699890
H	3.150268	-3.514137	-0.621408	H	2.482911	5.405682	1.613222
H	4.819362	-5.237495	-1.242814	H	2.065112	2.982767	1.974998
H	7.007739	-4.575901	-2.237238	C	0.005416	-2.230870	0.326152
H	7.490538	-2.158516	-2.610065	C	0.004275	-3.458134	-0.366007
H	5.811648	-0.435672	-1.995221	C	0.019523	-4.667965	0.328834
O	5.371947	1.556827	0.441234	C	0.036330	-4.691652	1.726135
C	6.044420	1.301213	1.669141	C	0.037762	-3.481977	2.423215
C	5.758941	-0.134217	2.059881	C	0.022843	-2.265937	1.736403
O	4.342955	-0.291969	2.120439	H	0.024761	-1.325687	2.286621
C	3.951126	-1.626332	2.458802	H	0.050399	-3.480283	3.511003
H	4.337860	-2.343298	1.725105	H	0.047906	-5.636621	2.261414
H	4.314848	-1.883652	3.462884	H	0.018189	-5.600634	-0.230004
H	2.860644	-1.652700	2.445919	H	-0.008119	-3.443444	-1.453144
H	6.178051	-0.824452	1.313933	O	-3.506410	-0.934835	-0.840546
H	6.212363	-0.350773	3.038815	Li	-3.643840	0.498541	0.347316
H	7.128775	1.442007	1.549002				

Table A1.5 (Continued).

Atom	X	Y	Z
O	-4.262422	-0.221684	2.182564
C	-5.677869	-0.049721	2.176119
C	-5.964227	1.382763	1.775948
O	-5.341384	1.613514	0.517067
C	-5.611221	2.908491	-0.019216
H	-5.060554	2.986591	-0.956456
H	-5.265736	3.693327	0.664745
H	-6.687527	3.024971	-0.204349
H	-5.565065	2.084235	2.524305
H	-7.051039	1.534188	1.699096
H	-6.094135	-0.247171	3.175410
H	-6.133202	-0.746267	1.457717
C	-3.871877	-1.554070	2.530035
H	-2.782921	-1.592731	2.478257
H	-4.200907	-1.789703	3.551272
H	-4.292128	-2.279661	1.823885
C	-4.407055	-1.872470	-1.127447
C	-5.681384	-1.528200	-1.637189
C	-6.631310	-2.508438	-1.923085
C	-6.350577	-3.861554	-1.713941
C	-5.094359	-4.217520	-1.216047
C	-4.136206	-3.246457	-0.924987
H	-3.159738	-3.531885	-0.539705
H	-4.854049	-5.266164	-1.051498
H	-7.092615	-4.622376	-1.940104
H	-7.600304	-2.211012	-2.319788
H	-5.896488	-0.477107	-1.816184
C	-2.022548	2.466229	-0.407446
C	-2.026953	3.531029	0.518036
C	-2.271703	4.839515	0.100693
C	-2.525584	5.124906	-1.243500
C	-2.524794	4.078476	-2.169334
C	-2.279348	2.766165	-1.762138
H	-2.282660	1.954413	-2.486572
H	-2.714067	4.282414	-3.220843
H	-2.711629	6.145642	-1.565191
H	-2.259497	5.643240	0.833510
H	-1.832455	3.308942	1.565090

Table A1.5 (Continued).

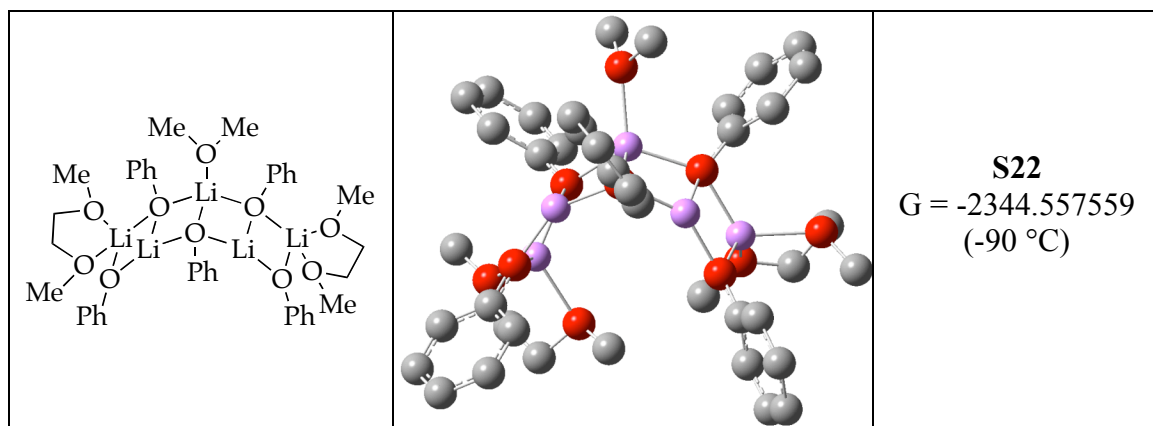
		<p style="text-align: center;">S21 G = -2189.593152 (-90 °C)</p>
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Atom	X	Y	Z	Atom	X	Y	Z
O	1.382046	-1.071584	-0.190871	H	7.744262	3.789347	-1.321799
Li	-0.007207	-0.313570	0.825823	H	7.249066	2.013004	-2.999219
O	0.246714	1.538169	0.406525	H	5.198872	0.622301	-2.783252
Li	1.660633	0.876982	-0.641248	Li	-1.674026	1.470725	0.319502
O	3.436222	0.811312	-0.853859	O	-1.864834	-0.361787	1.103552
Li	3.354454	-0.942896	-0.277457	Li	-3.343565	-0.349183	-0.162206
O	4.658176	-2.285294	-1.176784	O	-3.129995	1.410764	-0.711075
C	5.856738	-2.032279	-0.439032	C	-3.846902	2.058206	-1.626727
C	5.618806	-2.181984	1.058321	C	-3.670135	1.809943	-3.008258
O	4.485494	-1.381224	1.374066	C	-4.435925	2.480851	-3.962333
C	4.179851	-1.322364	2.760175	C	-5.400042	3.416296	-3.578355
H	3.300297	-0.684415	2.863603	C	-5.584815	3.672389	-2.216428
H	3.957364	-2.322290	3.158767	C	-4.826138	3.007780	-1.253826
H	5.013522	-0.884213	3.324771	H	-4.971842	3.205956	-0.194266
H	5.426407	-3.227974	1.342735	H	-6.329135	4.399914	-1.898353
H	6.504350	-1.834072	1.610776	H	-5.992591	3.938465	-4.324633
H	6.132685	-0.999327	-0.671391	H	-4.272729	2.272569	-5.018105
H	6.664684	-2.699004	-0.769952	H	-2.910439	1.091560	-3.308523
C	4.406716	-3.663200	-1.454282	O	-5.239692	-0.898832	0.375504
H	3.473317	-3.704832	-2.016147	C	-5.797954	-1.842437	-0.529316
H	5.223066	-4.080030	-2.058994	C	-5.023925	-1.711549	-1.835225
H	4.297505	-4.253880	-0.535562	O	-3.614455	-1.784935	-1.609302
C	4.521074	1.574670	-0.975394	C	-3.089871	-3.107461	-1.492613
C	5.428167	1.387084	-2.044263	H	-3.286367	-3.674958	-2.411655
C	6.573174	2.176531	-2.161844	H	-3.519239	-3.644876	-0.636521
C	6.853547	3.174473	-1.225353	H	-2.013263	-3.008166	-1.353797
C	5.962662	3.373273	-0.166139	H	-5.342818	-2.481336	-2.551505
C	4.816502	2.590490	-0.036995	H	-5.196508	-0.724884	-2.275307
H	4.123747	2.750873	0.786092	H	-6.862976	-1.629118	-0.706471
H	6.160762	4.150569	0.569352	H	-5.719079	-2.855776	-0.105997

Table A1.5 (Continued).

Atom	X	Y	Z
C	-5.878037	-0.865321	1.648072
H	-6.923591	-0.545429	1.545964
H	-5.840265	-1.851137	2.130424
H	-5.329614	-0.147748	2.259321
C	-2.183789	-0.837001	2.322848
C	-2.464097	0.032156	3.399938
C	-2.799895	-0.472377	4.657044
C	-2.867848	-1.850073	4.880682
C	-2.587436	-2.720899	3.824526
C	-2.249089	-2.227608	2.563101
H	-2.028155	-2.905651	1.741704
H	-2.630439	-3.796617	3.981667
H	-3.129656	-2.237596	5.861112
H	-3.009651	0.220767	5.468555
H	-2.409658	1.105949	3.233574
C	0.441177	2.693687	1.084888
C	0.043988	3.925722	0.526087
C	0.217351	5.116571	1.234012
C	0.791251	5.111679	2.506859
C	1.192867	3.895815	3.066381
C	1.020908	2.699933	2.369549
H	1.333564	1.754104	2.807442
H	1.643867	3.875702	4.055866
H	0.927590	6.040422	3.053310
H	-0.094571	6.054128	0.780371
H	-0.387171	3.933008	-0.473072
C	1.057020	-2.218395	-0.814758
C	0.878835	-3.415146	-0.084594
C	0.566424	-4.611477	-0.732350
C	0.423753	-4.654902	-2.122383
C	0.592663	-3.476050	-2.856136
C	0.902403	-2.274151	-2.217870
H	1.035395	-1.361599	-2.794106
H	0.481834	-3.488973	-3.938024
H	0.185162	-5.588254	-2.624442
H	0.437507	-5.517551	-0.144196
H	0.996798	-3.385073	0.996532

Table A1.5 (Continued).

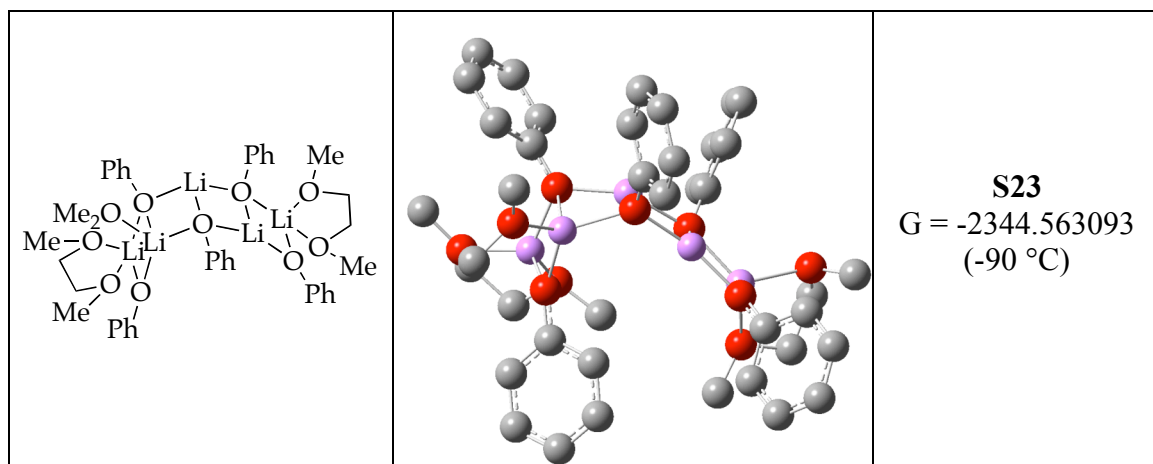


Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.492577	-1.601194	0.991045	H	2.583811	-0.794743	4.470291
O	0.192599	-0.086309	2.110527	C	1.572923	2.137293	-1.903099
Li	1.831211	-0.481460	1.253009	H	1.342080	2.860874	-2.696101
O	1.159093	-1.720255	-0.091340	H	0.683109	1.968910	-1.294362
Li	2.450189	-0.621122	-1.135119	H	2.385124	2.520608	-1.275821
O	3.235522	0.185947	0.345647	C	1.404776	-2.977170	-0.488035
C	4.204232	1.092997	0.424529	C	2.349425	-3.793138	0.176681
C	4.011302	2.327448	1.089371	C	2.592159	-5.100556	-0.246927
C	5.027960	3.280010	1.147142	C	1.909869	-5.638121	-1.342869
C	6.268748	3.043936	0.548643	C	0.975290	-4.842247	-2.011943
C	6.477892	1.826887	-0.105792	C	0.724661	-3.533260	-1.596921
C	5.469090	0.865871	-0.169231	H	-0.004702	-2.914218	-2.114578
H	5.640227	-0.088328	-0.662791	H	0.432440	-5.244207	-2.865073
H	7.441319	1.618784	-0.567946	H	2.100761	-6.657337	-1.666537
H	7.057824	3.789327	0.597479	H	3.321302	-5.705423	0.287773
H	4.846592	4.218570	1.667095	H	2.882461	-3.380808	1.030344
H	3.048406	2.517516	1.559006	Li	-1.149418	0.832603	1.156113
O	1.936674	0.874184	-2.484155	O	-2.081516	-0.621897	0.296431
C	3.090093	0.968545	-3.317964	Li	-2.497377	0.841009	-0.943069
H	2.899023	1.646052	-4.164200	O	-1.521563	2.153690	-0.055431
H	3.937343	1.359093	-2.737124	C	-1.580742	3.480690	-0.120363
C	3.401707	-0.420979	-3.834927	C	-1.443670	4.165381	-1.351732
O	3.567745	-1.276098	-2.710042	C	-1.518228	5.556493	-1.418549
C	3.972402	-2.599523	-3.054404	C	-1.732475	6.318321	-0.267380
H	4.955662	-2.580761	-3.543650	C	-1.870758	5.659075	0.957304
H	4.028630	-3.167552	-2.125838	C	-1.798875	4.269194	1.034327
H	3.238721	-3.072122	-3.719604	H	-1.915326	3.764833	1.991917
H	4.323341	-0.392847	-4.435045	H	-2.037939	6.233467	1.866137

Table A1.5 (Continued).

Atom	X	Y	Z	Atom	X	Y	Z
H	-1.787253	7.401844	-0.322263	H	-6.133156	-1.619390	2.112042
H	-1.403613	6.050718	-2.381567	H	-6.473747	-3.522081	0.537450
H	-1.266665	3.579214	-2.251225	H	-4.713570	-4.029861	-1.154887
O	-4.465594	1.329150	-1.279606	H	-2.645894	-2.656173	-1.260640
C	-4.897661	2.691831	-1.257259	C	0.416324	0.220361	3.404417
H	-4.519025	3.124494	-0.331075	C	0.216908	1.531500	3.887076
H	-4.492750	3.263905	-2.100795	C	0.451244	1.843866	5.225870
H	-5.994424	2.737731	-1.271454	C	0.898505	0.867839	6.120122
C	-4.825417	0.602861	-2.454396	C	1.112871	-0.429936	5.651967
H	-4.868423	-0.447877	-2.153342	C	0.876371	-0.755038	4.315120
H	-5.815966	0.909692	-2.816703	H	1.036390	-1.769842	3.956559
C	-3.777608	0.787282	-3.543318	H	1.467056	-1.201623	6.331850
O	-2.517751	0.450500	-2.968177	H	1.083651	1.116817	7.161040
C	-1.425654	0.573239	-3.873834	H	0.292075	2.863458	5.569408
H	-0.513014	0.351870	-3.318179	H	-0.100456	2.306678	3.191483
H	-1.534067	-0.135980	-4.705945	O	-0.991313	-3.218385	2.095466
H	-1.367437	1.594008	-4.277591	C	-1.191999	-4.528035	1.563879
H	-3.750647	1.825198	-3.908953	H	-0.923881	-5.285253	2.313380
H	-4.000533	0.128522	-4.396322	H	-2.238461	-4.663590	1.262422
C	-3.200806	-1.360356	0.367477	H	-0.539639	-4.630359	0.696724
C	-3.414900	-2.436928	-0.523586	C	-1.773696	-2.995480	3.268922
C	-4.579752	-3.204545	-0.458328	H	-1.510595	-3.729627	4.042998
C	-5.568418	-2.923634	0.488625	H	-2.844211	-3.066788	3.041176
C	-5.372828	-1.856680	1.371048	H	-1.537466	-1.993927	3.629994
C	-4.211668	-1.085705	1.315446				
H	-4.069314	-0.252760	2.000474				

Table A1.5 (Continued).

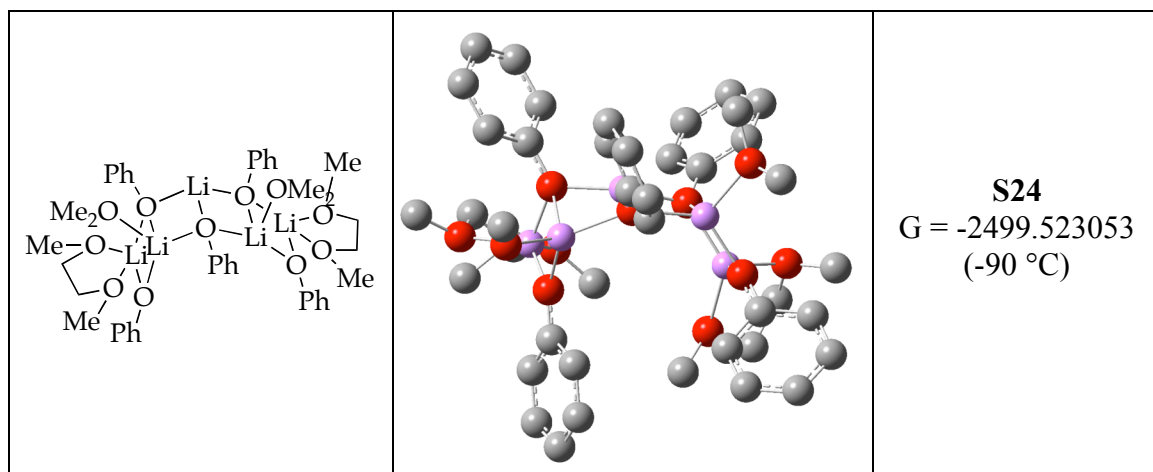


Atom	X	Y	Z	Atom	X	Y	Z
Li	1.391799	-1.008202	-0.590160	C	4.500623	1.297916	3.058176
O	-0.289811	-1.380076	-1.319307	O	3.381045	1.585371	2.223298
Li	-1.672727	0.006652	-1.646733	C	3.519012	2.807127	1.494917
O	-2.549468	-0.309106	0.224236	H	2.638091	2.904932	0.858322
Li	-0.871125	-1.070883	0.490448	H	3.576533	3.660081	2.184477
O	0.881375	-0.783074	1.316262	H	4.416086	2.781867	0.864392
Li	2.735560	-0.162681	1.323296	H	5.421626	1.302371	2.456458
O	3.105301	-0.468682	-0.465190	H	4.601236	2.060301	3.845869
C	4.174646	-0.288663	-1.237965	C	0.635576	-1.608345	2.355033
C	4.549203	0.997172	-1.694484	C	0.383189	-1.097387	3.648370
C	5.681742	1.177761	-2.488976	C	0.105571	-1.953749	4.713522
C	6.478767	0.091531	-2.858881	C	0.063022	-3.338789	4.526503
C	6.116099	-1.186845	-2.424573	C	0.303380	-3.856577	3.252538
C	4.987187	-1.378613	-1.629042	C	0.587088	-3.009273	2.178914
H	4.703897	-2.375726	-1.299141	H	0.789086	-3.421844	1.192207
H	6.718534	-2.047115	-2.709471	H	0.276083	-4.931062	3.087610
H	7.358444	0.236553	-3.479746	H	-0.156339	-4.001329	5.358773
H	5.939774	2.179239	-2.827999	H	-0.084855	-1.533712	5.698886
H	3.918825	1.841468	-1.427870	H	0.399154	-0.019890	3.792488
O	4.010087	-1.047864	2.667427	Li	-2.431003	1.588231	0.369072
C	5.184788	-1.665519	2.133543	O	-1.399686	1.808519	-1.161128
H	4.844137	-2.377235	1.381999	C	-0.638190	2.825094	-1.541389
H	5.849070	-0.938069	1.651591	C	0.702371	2.638106	-1.964013
H	5.725590	-2.194215	2.929121	C	1.493591	3.718505	-2.354136
C	4.252421	-0.069417	3.676953	C	0.991473	5.024159	-2.335399
H	3.346450	-0.044738	4.289909	C	-0.329500	5.226997	-1.927888
H	5.098968	-0.364139	4.311820	C	-1.132410	4.153453	-1.540578

Table A1.5 (Continued).

Atom	X	Y	Z	Atom	X	Y	Z
H	-2.168603	4.315832	-1.249263	H	-3.228594	-0.886797	2.701664
H	-0.745544	6.232960	-1.918987	H	-5.382731	-1.903559	3.400687
H	1.611471	5.861352	-2.643862	H	-7.110254	-2.486228	1.700337
H	2.513168	3.532778	-2.685976	H	-6.641791	-2.050012	-0.708420
H	1.103763	1.627481	-1.984952	H	-4.481990	-1.033797	-1.402025
O	-1.628162	2.533587	2.024059	O	-2.699520	-0.068333	-3.364422
C	-2.365610	3.740509	2.178768	C	-2.967451	-1.168222	-4.229298
H	-2.127303	4.217882	3.141448	H	-2.410705	-1.064586	-5.170158
H	-2.111747	4.438945	1.368073	H	-4.042712	-1.226543	-4.452474
C	-3.836510	3.381285	2.138176	H	-2.645728	-2.074458	-3.715101
O	-4.086130	2.694539	0.915891	C	-3.067555	1.184574	-3.936649
C	-5.439487	2.256576	0.790754	H	-4.143630	1.202325	-4.160622
H	-6.116748	3.120117	0.742348	H	-2.822997	1.949027	-3.199479
H	-5.505452	1.678590	-0.130980	H	-2.504349	1.366425	-4.862500
H	-5.718092	1.610938	1.632708	C	-0.389258	-2.513941	-2.040767
H	-4.446415	4.295294	2.196666	C	0.453801	-2.741605	-3.149956
H	-4.095459	2.731977	2.987444	C	0.353440	-3.917335	-3.894765
C	-0.213116	2.734053	2.047975	C	-0.587983	-4.896011	-3.563213
H	0.093959	3.155569	3.015521	C	-1.430779	-4.679918	-2.470489
H	0.243670	1.752834	1.908735	C	-1.338517	-3.507514	-1.716985
H	0.093857	3.404441	1.236072	H	-2.004649	-3.344955	-0.872210
C	-3.706084	-0.878937	0.599728	H	-2.171139	-5.428710	-2.197848
C	-4.691222	-1.223084	-0.351751	H	-0.662211	-5.810276	-4.145120
C	-5.901071	-1.793240	0.046055	H	1.016549	-4.066299	-4.743890
C	-6.168197	-2.039048	1.395899	H	1.177172	-1.975490	-3.420637
C	-5.197408	-1.710508	2.346210				
C	-3.983795	-1.138808	1.960221				

Table A1.5 (Continued).

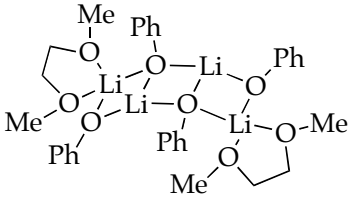
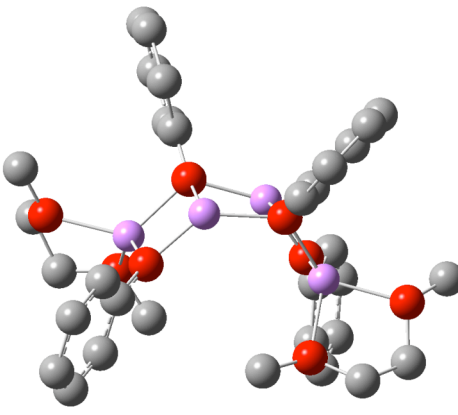


Atom	X	Y	Z	Atom	X	Y	Z
Li	1.647308	1.072248	-1.037436	H	4.401909	-4.514961	-1.389404
O	-0.048857	1.740842	-0.203628	C	3.574604	-3.679628	0.429428
Li	-1.508728	1.192720	1.106410	O	2.458367	-2.856719	0.751810
O	-2.507190	0.116624	-0.358067	C	2.402922	-2.519462	2.145139
Li	-0.762054	0.211559	-1.049527	H	1.514122	-1.908317	2.297505
O	0.780925	-0.680888	-1.655034	H	2.326117	-3.430841	2.752005
Li	2.342013	-1.341960	-0.692738	H	3.291478	-1.948155	2.437461
O	3.104965	0.254162	-0.203626	H	4.504987	-3.187244	0.750310
C	4.031528	0.682022	0.643591	H	3.503746	-4.647569	0.949933
C	3.728422	0.946649	2.003003	C	0.607332	-1.281336	-2.848922
C	4.708340	1.397746	2.885905	C	-0.375337	-2.281355	-3.022240
C	6.023695	1.604845	2.458716	C	-0.559363	-2.898420	-4.260977
C	6.340891	1.353021	1.121924	C	0.227264	-2.545778	-5.359531
C	5.369152	0.900145	0.228169	C	1.206461	-1.561195	-5.198612
H	5.621504	0.713155	-0.813346	C	1.398010	-0.936095	-3.966745
H	7.357604	1.512148	0.766859	H	2.163260	-0.174290	-3.841467
H	6.782625	1.957934	3.151482	H	1.830176	-1.274438	-6.042864
H	4.439830	1.590671	3.923023	H	0.080943	-3.027634	-6.322181
H	2.708439	0.785127	2.342345	H	-1.325931	-3.663810	-4.365958
O	3.560418	-2.642619	-1.764823	H	-0.988795	-2.561672	-2.168689
C	4.861392	-2.127035	-2.052220	Li	-2.564998	-1.268476	0.946593
H	4.708846	-1.194951	-2.596932	O	-1.444018	-0.408992	2.135097
H	5.428248	-1.913953	-1.138049	C	-0.832265	-0.770019	3.252996
H	5.417112	-2.835416	-2.680899	C	0.144848	0.056163	3.863747
C	3.553890	-3.891181	-1.075160	C	0.797712	-0.337297	5.031387
H	2.626072	-4.393211	-1.367480	C	0.507225	-1.561598	5.641302

Table A1.5 (Continued).

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.463813	-2.383798	5.062234	O	-2.515459	2.530833	2.274083
C	-1.123638	-2.000159	3.895712	C	-2.572409	3.954795	2.235869
H	-1.887087	-2.642069	3.459179	H	-2.084040	4.382334	3.122147
H	-0.714867	-3.335548	5.527367	H	-3.617691	4.294511	2.203964
H	1.018419	-1.862901	6.551347	H	-2.052201	4.281248	1.336639
H	1.545299	0.321573	5.468659	C	-3.181882	1.996525	3.415050
H	0.383186	1.007938	3.393748	H	-4.250756	2.255628	3.390760
O	-2.210052	-3.183569	0.284845	H	-3.048966	0.915544	3.378504
C	-3.364083	-3.997347	0.459322	H	-2.740329	2.388752	4.341132
H	-3.399124	-4.786344	-0.306783	C	-0.101218	3.076659	-0.305207
H	-3.337724	-4.473970	1.450862	C	0.806293	3.891038	0.411708
C	-4.584497	-3.106500	0.344830	C	0.756531	5.281668	0.309770
O	-4.444157	-2.074135	1.318769	C	-0.195396	5.908225	-0.501618
C	-5.617331	-1.273658	1.470030	C	-1.101866	5.115581	-1.211912
H	-6.464457	-1.897806	1.785441	C	-1.061402	3.722701	-1.118534
H	-5.397291	-0.542930	2.250268	H	-1.778739	3.113626	-1.664209
H	-5.862560	-0.750600	0.538775	H	-1.853061	5.583302	-1.845055
H	-5.490157	-3.699111	0.541071	H	-0.230723	6.991472	-0.577082
H	-4.660519	-2.665190	-0.659506	H	1.467899	5.881316	0.873847
C	-0.987224	-3.880428	0.521485	H	1.544430	3.406288	1.046856
H	-0.894796	-4.734178	-0.163522	O	2.289151	2.275464	-2.542191
H	-0.174369	-3.178314	0.338401	C	1.441463	2.776489	-3.571712
H	-0.938556	-4.233274	1.559941	H	2.023076	2.966285	-4.485241
C	-3.559132	0.436060	-1.126451	H	0.695311	2.006491	-3.777394
C	-4.478804	1.431597	-0.725557	H	0.941092	3.699589	-3.255058
C	-5.578360	1.754193	-1.521191	C	3.351361	3.174375	-2.226596
C	-5.799776	1.101090	-2.737244	H	3.977307	3.349690	-3.113261
C	-4.894897	0.119534	-3.148706	H	3.949104	2.702814	-1.445066
C	-3.791735	-0.213699	-2.360513	H	2.955043	4.131531	-1.864044
H	-3.086804	-0.973042	-2.692329				
H	-5.044505	-0.394013	-4.096140				
H	-6.656037	1.357744	-3.354651				
H	-6.267457	2.527782	-1.188131				
H	-4.302445	1.944143	0.217094				

Table A1.5 (Continued).

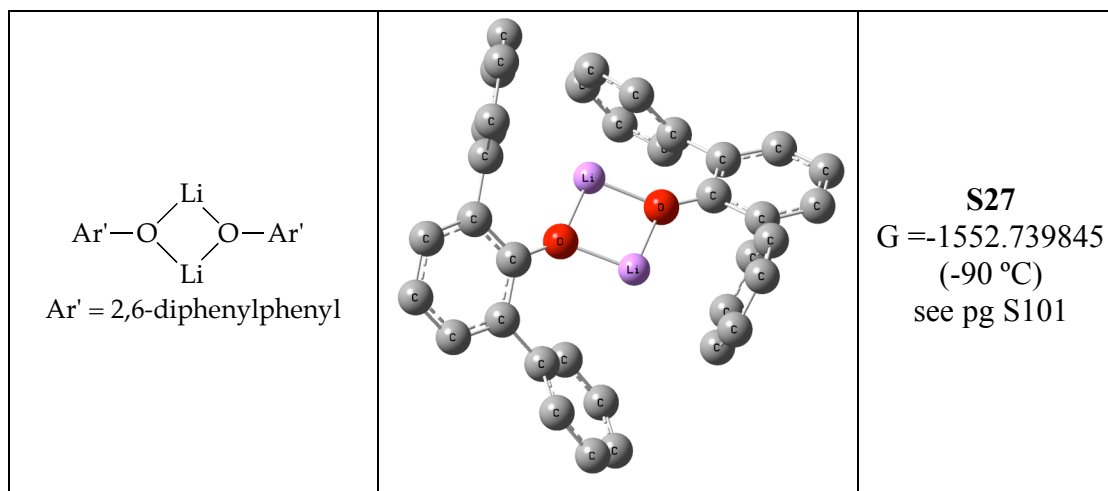
		<p>S25 G = -1875.179010 (-90 °C) see pg S101</p>
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Atom	X	Y	Z	Atom	X	Y	Z
Li	0.645265	1.213883	0.810355	H	5.625845	-1.935603	-1.170834
O	-1.206640	0.991174	1.180681	H	4.395891	-2.505417	-0.001876
Li	-0.635759	-0.881792	1.124715	C	5.116109	0.033989	0.518091
O	1.236051	-0.597271	1.192369	H	6.166629	0.010762	0.199163
Li	2.260416	-0.286838	-0.438329	H	4.804853	1.069304	0.665847
O	1.661951	1.465729	-0.676260	H	4.998975	-0.526790	1.453908
C	2.089362	2.445160	-1.467353	C	1.876654	-1.306257	2.138901
C	2.150812	2.284544	-2.872023	C	2.390288	-0.687735	3.299123
C	2.592922	3.317306	-3.698372	C	3.056851	-1.433823	4.271593
C	2.988002	4.545206	-3.161661	C	3.232565	-2.812133	4.121449
C	2.935230	4.720473	-1.775900	C	2.725264	-3.437264	2.979540
C	2.497097	3.693965	-0.941070	C	2.057847	-2.700991	1.999056
H	2.468252	3.834570	0.138267	H	1.667177	-3.186447	1.107776
H	3.241906	5.668133	-1.337490	H	2.846300	-4.510507	2.848419
H	3.331105	5.347881	-3.808464	H	3.749268	-3.388549	4.883562
H	2.627446	3.160052	-4.774826	H	3.438520	-0.931401	5.157701
H	1.838026	1.332100	-3.296295	H	2.249272	0.383757	3.425191
O	4.275626	-0.496855	-0.505788	O	-1.884317	-1.447679	-0.058835
C	4.574358	-1.842981	-0.861143	Li	-2.448643	0.344594	-0.136776
C	3.664811	-2.208213	-2.018682	O	-4.483743	0.486818	-0.130120
O	2.325913	-1.957208	-1.606416	C	-5.223434	-0.581976	0.462472
C	1.346082	-2.318483	-2.578968	H	-4.858463	-0.684510	1.485286
H	1.481629	-1.738806	-3.502877	H	-6.294644	-0.340807	0.479169
H	1.411172	-3.389738	-2.809483	H	-5.058155	-1.519401	-0.082383
H	0.368161	-2.105219	-2.146027	C	-4.876557	0.770313	-1.469970
H	3.905109	-1.599296	-2.903293	H	-4.771173	-0.133084	-2.088259
H	3.795332	-3.269568	-2.276523	H	-5.925214	1.101376	-1.502480

Table A1.5 (Continued).

Atom	X	Y	Z
C	-3.970801	1.872972	-1.981462
O	-2.628801	1.418216	-1.847673
C	-1.652195	2.369869	-2.276525
H	-1.767599	3.317092	-1.733267
H	-0.672155	1.945466	-2.057982
H	-1.747254	2.555656	-3.354318
H	-4.202972	2.091441	-3.034419
H	-4.114401	2.791692	-1.393072
C	-2.228174	-2.507632	-0.779321
C	-2.493709	-2.401820	-2.167700
C	-2.858060	-3.519368	-2.919840
C	-2.972548	-4.778121	-2.324696
C	-2.715274	-4.899140	-0.955389
C	-2.352401	-3.790421	-0.193434
H	-2.161335	-3.890166	0.873282
H	-2.800871	-5.870675	-0.472581
H	-3.256094	-5.645958	-2.913657
H	-3.052454	-3.403756	-3.984731
H	-2.395888	-1.424915	-2.637398
C	-1.668201	1.775007	2.173878
C	-1.516564	3.177494	2.119351
C	-1.983422	3.988857	3.154639
C	-2.618189	3.431847	4.266812
C	-2.780259	2.045262	4.329113
C	-2.314783	1.225532	3.301535
H	-2.440901	0.145690	3.357185
H	-3.271710	1.594112	5.188286
H	-2.980492	4.066111	5.070810
H	-1.851978	5.066562	3.086778
H	-1.037379	3.617291	1.246090

Table A1.5 (Continued).

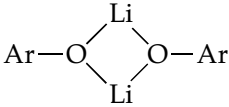
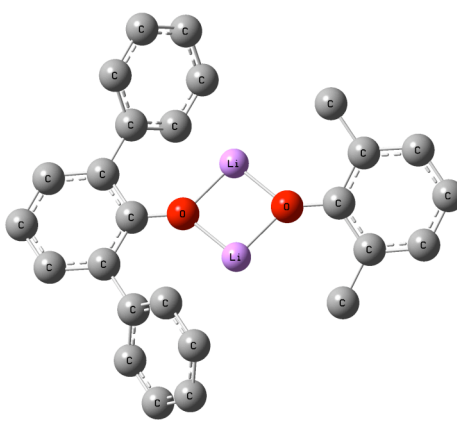


Atom	X	Y	Z	Atom	X	Y	Z
C	-2.664969	2.442608	0.296970	C	4.793478	-1.490679	0.005188
C	-2.371815	1.168845	-0.268623	C	4.749091	-2.691575	0.712091
C	-3.441076	0.421802	-0.848147	H	5.654334	-3.268653	0.876347
C	-4.737984	0.954374	-0.839545	C	3.523630	-3.141035	1.202602
C	-5.017099	2.196306	-0.274220	C	2.348002	-2.416000	0.985417
C	-3.976289	2.928913	0.294863	C	1.041940	-2.923473	1.491440
H	-4.173189	3.905746	0.730958	C	0.789837	-3.034865	2.867260
H	-6.027587	2.593925	-0.289412	H	1.568467	-2.748854	3.569088
H	-5.538263	0.385515	-1.306893	C	-0.443536	-3.491449	3.338531
C	-3.201826	-0.923731	-1.432953	C	-1.456900	-3.841929	2.445043
C	-2.103124	-1.184676	-2.278454	C	-1.221611	-3.753731	1.070229
C	-1.913384	-2.445637	-2.847989	H	-1.991272	-4.042220	0.360060
C	-2.817170	-3.480953	-2.592552	C	0.017977	-3.305544	0.601268
C	-3.912738	-3.238888	-1.761050	H	0.214528	-3.291400	-0.470520
C	-4.096856	-1.980881	-1.184876	H	-2.417442	-4.190582	2.813968
H	-4.942904	-1.811006	-0.524626	H	-0.614765	-3.565438	4.409487
H	-4.626378	-4.033104	-1.555507	H	3.466524	-4.081114	1.747036
H	-2.672853	-4.459785	-3.041873	H	5.741912	-1.124053	-0.381172
H	-1.066985	-2.612419	-3.509998	C	3.735569	0.558400	-0.959018
H	-1.414169	-0.378959	-2.511266	C	4.175279	0.568720	-2.291909
O	-1.147232	0.672765	-0.201904	C	4.302644	1.764503	-3.001595
Li	-0.481588	-1.025452	0.023675	C	3.997796	2.981144	-2.389979
O	1.278583	-0.475058	0.095085	C	3.567083	2.990209	-1.061041
Li	0.594304	1.214619	-0.024510	C	3.430121	1.792174	-0.355506
C	2.386710	-1.174265	0.287254	H	3.142986	1.810932	0.694788
C	3.643138	-0.720526	-0.202912	H	3.365326	3.934540	-0.562797

Table A1.5 (Continued).

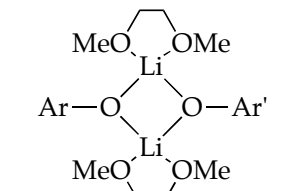
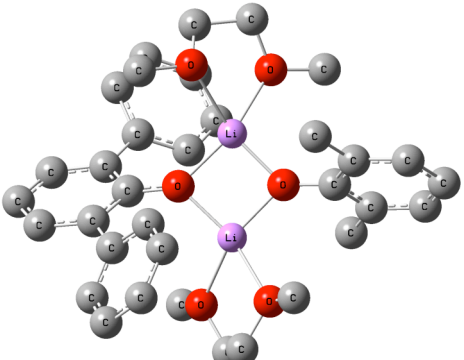
Atom	X	Y	Z
H	4.106142	3.913750	-2.937047
H	4.643380	1.744424	-4.033720
H	4.414755	-0.375958	-2.772731
C	-1.576467	3.237587	0.925698
C	-1.648819	3.612839	2.276320
C	-0.643894	4.381419	2.867810
C	0.458603	4.796640	2.119982
C	0.543873	4.440489	0.771321
C	-0.458229	3.664479	0.182564
H	-0.414144	3.439222	-0.882378
H	1.376220	4.789932	0.167221
H	1.236732	5.401781	2.576991
H	-0.723883	4.655921	3.916565
H	-2.502354	3.289030	2.865613

Table A1.5 (Continued).

 <p>Ar' = 2,6-diphenylphenyl Ar = 2,6-dimethylphenyl</p>		<p>S28 G = -1169.361703 (-90 °C) see pg S101</p>
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Atom	X	Y	Z	Atom	X	Y	Z
C	-3.169700	-2.425565	0.693442	C	2.350255	-3.543277	0.766719
C	-3.936463	-1.177658	0.334405	H	3.099602	-3.392299	1.539041
C	-3.220550	-0.001376	0.000083	C	1.646898	-4.749194	0.705420
C	-3.935775	1.175124	-0.334888	C	0.666486	-4.948019	-0.267579
C	-5.332280	1.155522	-0.331182	C	0.405407	-3.932601	-1.193526
C	-6.039692	-0.000885	-0.001201	H	-0.331788	-4.086032	-1.978125
C	-5.332939	-1.157552	0.329423	C	1.113771	-2.728871	-1.134733
H	-5.873827	-2.065748	0.590093	H	0.942614	-1.961918	-1.887299
H	-7.126094	-0.000736	-0.001685	H	0.119438	-5.885429	-0.313671
H	-5.872577	2.063936	-0.592332	H	1.862997	-5.533389	1.426415
C	-3.168208	2.422697	-0.693113	H	4.779953	-2.142230	-0.115769
H	-2.554473	2.787828	0.146726	H	4.777740	2.146459	0.113019
H	-2.491248	2.255997	-1.545270	C	2.095142	2.508629	0.146801
H	-3.841049	3.241127	-0.969424	C	2.345887	3.544895	-0.766867
O	-1.886575	-0.001487	0.000690	C	1.641448	4.750151	-0.704914
Li	-0.546837	-1.240470	0.023393	C	0.661752	4.948042	0.268985
O	0.793487	-0.000112	0.000971	C	0.402462	3.932350	1.195141
Li	-0.548194	1.239138	-0.021856	C	1.111887	2.729285	1.135687
C	2.112614	0.000672	0.000163	H	0.942096	1.962132	1.888352
C	2.839742	1.223574	0.074104	H	-0.334184	4.085073	1.980391
C	4.238748	1.203317	0.055886	H	0.113868	5.884938	0.315617
C	4.945501	0.002213	-0.001432	H	1.856159	5.534545	-1.426109
H	6.031397	0.002820	-0.002019	H	3.094664	3.394655	-1.539887
C	4.240006	-1.199674	-0.058008	H	-2.555181	-2.790879	-0.145730
C	2.841015	-1.221426	-0.074680	H	-2.493603	-2.259078	1.546292
C	2.097673	-2.507255	-0.146713	H	-3.843228	-3.243695	0.968961

Table A1.5 (Continued).

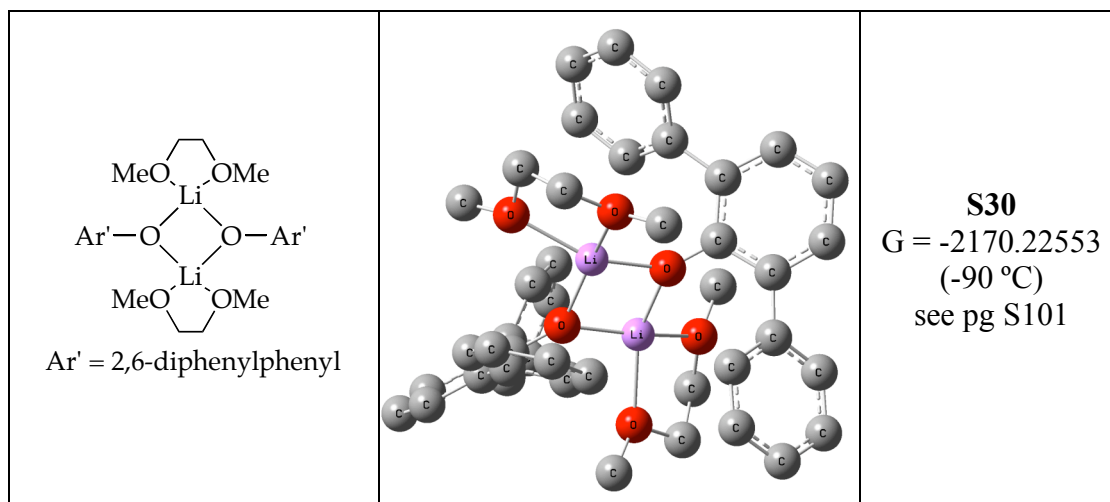
 <p>Ar = 2,6-diphenylphenyl Ar' = 2,6-dimethylphenyl</p>		<p>S29 G = -1786.854325 (-90 °C) see pg S101</p>
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Atom	X	Y	Z	Atom	X	Y	Z
C	2.922316	0.881726	2.547005	H	0.117633	4.998937	1.608584
C	3.707459	0.889940	1.258510	C	1.811391	3.882882	0.189370
C	3.032446	0.631589	0.032396	H	1.524976	4.808744	0.327932
C	3.780214	0.643319	1.178697	H	2.559838	4.112587	0.959746
C	5.152898	0.906210	1.140702	H	2.243268	3.170374	0.511548
C	5.813195	1.163113	0.061665	C	2.192752	0.483567	0.013488
C	5.080262	1.152117	1.249462	C	3.171579	0.456398	0.461125
H	5.582971	1.350257	2.195272	C	4.523738	0.085865	0.521210
H	6.880421	1.367880	0.073119	C	4.959698	1.175595	0.128428
H	5.712416	0.909654	2.075292	H	6.012066	1.439385	0.181174
C	3.073869	0.362153	2.482730	C	4.020505	2.092951	0.334717
H	2.270967	1.084072	2.684234	C	2.655071	1.784690	0.412472
H	2.593961	0.626309	2.479730	C	1.728311	2.832195	0.920446
H	3.774317	0.395210	3.324620	C	1.927296	4.182608	0.570124
O	1.728396	0.390011	0.017323	H	2.713905	4.433694	0.136066
Li	0.652695	1.016296	0.621153	C	1.137676	5.201052	1.104502
O	0.920346	0.164964	0.078430	C	0.112951	4.899863	2.004487
Li	0.224422	1.237293	0.697256	C	0.113545	3.565532	2.350202
O	0.666922	3.262907	0.769247	H	0.902246	3.311729	3.054806
C	0.156298	3.970231	1.888403	C	0.675145	2.547896	1.811020
C	1.071337	3.235974	2.383002	H	0.483136	1.518656	2.087727
O	0.701638	1.879073	2.609739	H	0.497620	5.691813	2.430506
C	1.763241	1.116537	3.179464	H	1.325616	6.232926	0.816798
H	2.624303	1.068951	2.501709	H	4.353461	3.071613	0.671624
H	1.382122	0.108716	3.345580	H	5.243090	0.803099	0.909048
H	2.072346	1.550556	4.140906	C	2.799651	1.831532	0.894734
H	1.424866	3.699624	3.317048	C	3.622892	2.924951	0.558275
H	1.878481	3.286100	1.638745	C	3.344242	4.215782	1.009636
H	0.922660	4.016464	2.677610	C	2.226346	4.454846	1.811098

Table A1.5 (Continued).

Atom	X	Y	Z
C	1.392820	3.386376	2.147856
C	1.670838	2.097444	1.692986
H	1.010351	1.282377	1.963340
H	0.520085	3.553817	2.774735
H	2.009318	5.457937	2.169173
H	4.003696	5.035307	0.733376
H	4.493130	2.756823	0.070801
O	2.073624	2.546096	0.946687
C	1.509448	3.623229	1.682715
C	0.738509	3.021167	2.839912
O	0.173803	2.072735	2.305300
C	1.046733	1.522526	3.284918
H	1.611918	2.319255	3.788101
H	1.742372	0.867488	2.760850
H	0.485482	0.950535	4.038004
H	0.199026	3.814302	3.379795
H	1.425643	2.526004	3.543870
H	2.302096	4.279001	2.074129
H	0.846621	4.217123	1.037884
C	3.031668	2.961455	0.024253
H	2.565281	3.606227	0.780100
H	3.854502	3.502991	0.462828
H	3.421852	2.055048	0.487332
H	2.472468	0.101489	2.739776
H	2.090865	1.599675	2.523278
H	3.562594	1.131912	3.400262

Table A1.5 (Continued).

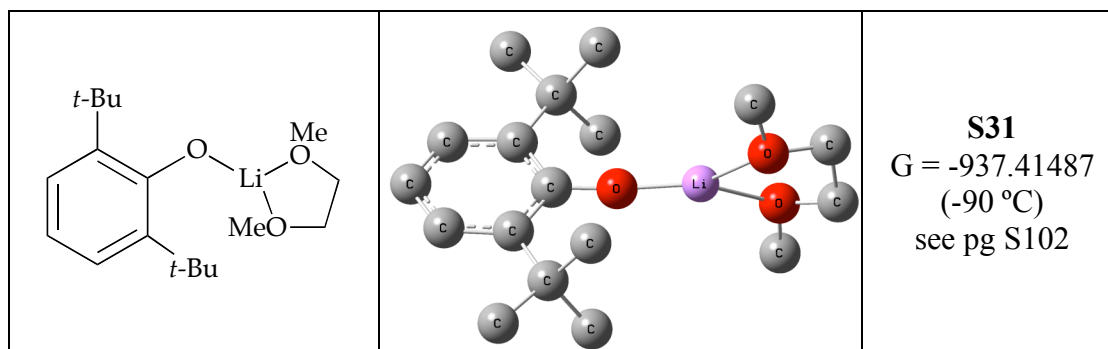


Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.000543	-1.345001	-0.001585	C	2.699098	3.539820	-3.441718
O	-1.352142	0.001204	-0.000303	C	1.630158	3.027726	-4.179925
Li	0.000661	1.345772	0.003453	C	1.115672	1.772121	-3.846509
O	1.352585	-0.000337	0.002233	C	1.661894	1.038203	-2.792367
C	2.666593	-0.002825	0.002736	H	1.255828	0.063233	-2.550983
C	3.413854	0.732515	-0.980323	H	0.290270	1.354286	-4.418782
C	4.815891	0.710496	-0.954256	H	1.207880	3.595209	-5.005302
C	5.524303	-0.008822	0.003689	H	3.111785	4.516320	-3.684596
H	6.610534	-0.011108	0.004040	H	4.071573	3.217110	-1.819357
C	4.812259	-0.725205	0.961157	O	-1.083556	3.001697	-0.775687
C	3.410158	-0.741312	0.986270	C	-1.949784	2.977635	-1.905148
C	2.740402	-1.537209	2.050994	H	-1.377696	3.052991	-2.839130
C	1.655853	-1.039711	2.797167	H	-2.670068	3.806057	-1.851618
H	1.254349	-0.062822	2.555905	H	-2.489735	2.031330	-1.871561
C	1.105826	-1.771542	3.850803	C	-0.338576	4.208546	-0.668734
C	1.614484	-3.029557	4.184046	C	0.346926	4.206063	0.682090
C	2.681419	-3.546301	3.446171	O	1.087398	2.996279	0.787123
H	3.089544	-4.524743	3.688946	C	1.950909	2.965869	1.918499
C	3.232099	-2.810770	2.395988	H	2.674053	3.792049	1.869191
H	4.056153	-3.229230	1.824555	H	1.376787	3.040126	2.851337
H	1.189261	-3.595368	5.009058	H	2.487791	2.017877	1.883181
H	0.282028	-1.350195	4.422811	H	1.019664	5.074844	0.750791
H	5.351996	-1.272397	1.730426	H	-0.390728	4.264963	1.494915
H	5.358434	1.255331	-1.723217	H	0.399082	4.266329	-1.481618
C	2.748294	1.530998	-2.045760	H	-1.008073	5.079981	-0.735675
C	3.245930	2.802134	-2.391041	C	-2.666153	0.001926	-0.000744

Table A1.5 (Continued).

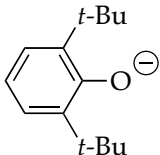
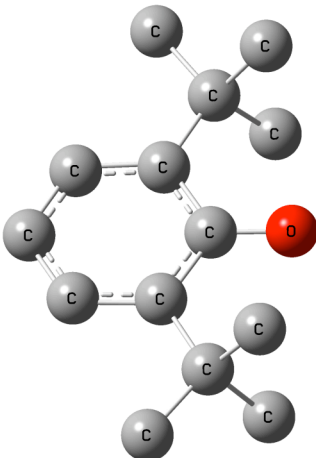
Atom	X	Y	Z	Atom	X	Y	Z
C	-3.411663	-0.728414	-0.988887	H	-1.019557	-5.078316	0.727229
C	-4.813723	-0.708833	-0.963469	C	-1.953844	-2.975891	1.903659
C	-5.523820	0.003372	-0.001444	H	-1.380125	-3.054533	2.836381
H	-6.610055	0.003867	-0.001682	H	-2.491414	-2.028122	1.872852
C	-4.813492	0.715041	0.960790	H	-2.676375	-3.802336	1.849822
C	-3.411417	0.733292	0.986797				
C	-2.743515	1.524057	2.056547				
C	-1.658564	1.023963	2.800374				
C	-1.109951	1.750617	3.858305				
C	-1.620461	3.006046	4.198382				
H	-1.196325	3.567844	5.026690				
C	-2.687872	3.525369	3.463031				
H	-3.097486	4.501855	3.711105				
C	-3.237166	2.794908	2.408583				
H	-4.061626	3.215410	1.839229				
H	-0.285783	1.327217	4.428266				
H	-1.255505	0.049042	2.553801				
H	-5.354549	1.256685	1.733056				
H	-5.354963	-1.249761	-1.736108				
C	-2.744090	-1.519036	-2.058954				
C	-1.658268	-1.019333	-2.801787				
C	-1.110214	-1.745278	-3.860495				
C	-1.622162	-2.999630	-4.202373				
H	-1.198509	-3.560800	-5.031353				
C	-2.690363	-3.518646	-3.467927				
C	-3.239126	-2.788867	-2.412718				
H	-4.064292	-3.209084	-1.844175				
H	-3.101286	-4.494184	-3.717579				
H	-0.285335	-1.322153	-4.429637				
H	-1.254032	-0.045269	-2.553764				
O	-1.089695	-3.000002	0.772624				
C	-0.347745	-4.208468	0.662742				
C	0.338295	-4.204270	-0.687786				
O	1.082110	-2.996188	-0.789310				
C	1.947336	-2.965693	-1.919406				
H	2.667271	-3.794757	-1.871521				
H	2.487785	-2.019858	-1.880562				
H	1.374269	-3.035069	-2.853243				
H	1.008857	-5.074595	-0.758308				
H	-0.399098	-4.259269	-1.501023				
H	0.389363	-4.270130	1.475868				

Table A1.5 (Continued).



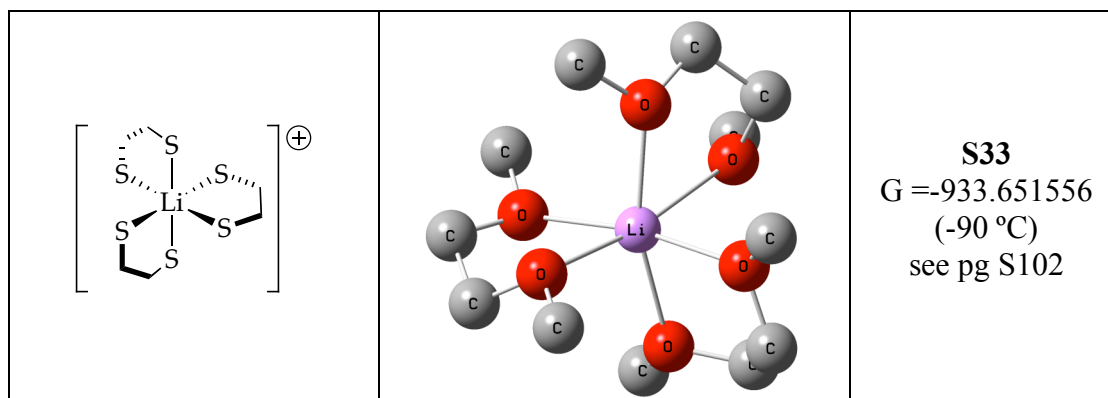
Atom	X	Y	Z	Atom	X	Y	Z
C	-4.350731	-0.082719	-0.843778	C	0.348567	2.784268	1.171626
H	-4.398580	0.957869	-1.197646	H	1.022765	2.891982	2.029933
H	-5.193713	-0.639529	-1.277073	H	-0.283331	3.682266	1.124438
C	-4.418833	-0.135722	0.670973	H	-0.283667	1.911345	1.346298
H	-5.302839	0.412851	1.025804	C	0.220693	2.635130	-1.362455
H	-4.487696	-1.176567	1.020459	H	0.803612	2.604390	-2.290950
O	-3.224416	0.463341	1.167771	H	-0.446011	1.769873	-1.357039
Li	-1.688627	-0.083812	0.032261	H	-0.385316	3.551941	-1.374765
O	-3.110567	-0.669183	-1.230942	H	3.885790	2.280685	-0.267883
C	-2.912675	-0.730110	-2.645393	C	1.436160	-2.553821	0.218978
H	-1.929067	-1.173475	-2.804529	C	2.462079	-3.706604	0.266050
H	-3.682588	-1.358087	-3.111071	H	3.147621	-3.613637	1.116038
H	-2.941525	0.274875	-3.086327	H	1.931887	-4.661109	0.373513
O	-0.003008	-0.032629	0.094986	H	3.060801	-3.763242	-0.650250
C	1.312322	0.032060	0.026469	C	0.626377	-2.624817	1.536765
C	2.104217	-1.167517	0.074690	H	1.296782	-2.540589	2.400592
C	3.495980	-1.059609	-0.009240	H	-0.098239	-1.809830	1.591238
H	4.108445	-1.954272	0.023109	H	0.095550	-3.583998	1.615252
C	4.136260	0.169804	-0.134200	C	0.513894	-2.834181	-0.992580
H	5.220237	0.222565	-0.197684	H	1.100426	-2.866414	-1.918880
C	3.370158	1.330993	-0.173376	H	0.007199	-3.802809	-0.879693
C	1.974140	1.303143	-0.094571	H	-0.240199	-2.051197	-1.096167
C	1.163916	2.618695	-0.134325	C	-3.159645	0.538051	2.593421
C	2.062718	3.867977	-0.254459	H	-2.198632	0.991412	2.839248
H	2.751995	3.960713	0.592446	H	-3.974245	1.163389	2.979802
H	2.654808	3.863029	-1.176797	H	-3.221643	-0.463418	3.039049
H	1.435591	4.768062	-0.269339				

Table A1.5 (Continued).

		<p>S32 G = -621.110315 (-90 °C) see pg S102</p>
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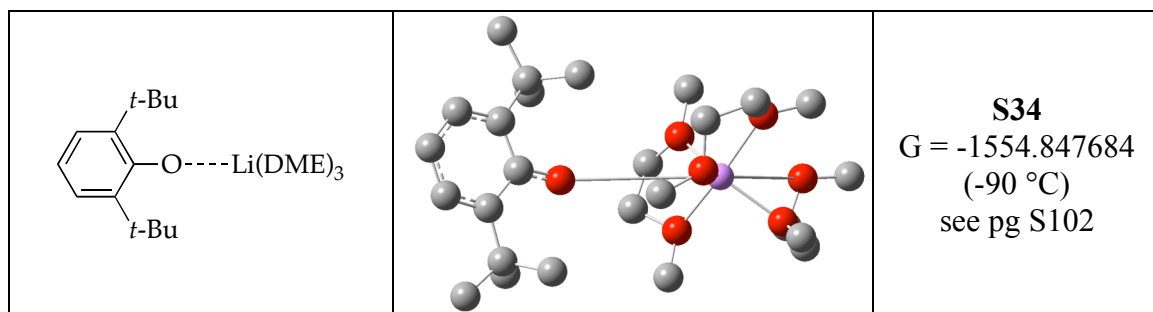
Atom	X	Y	Z	Atom	X	Y	Z
C	2.580348	-0.309132	-0.000034	H	-3.589815	-1.807391	-1.251249
C	1.242466	0.457692	0.000044	C	-2.668761	-1.203950	1.260778
C	0.000004	-0.304851	0.000165	H	-2.677889	-0.586859	2.169310
C	-1.242463	0.457686	0.000014	H	-3.590084	-1.807085	1.251339
C	-1.201859	1.851771	0.000041	H	-1.799915	-1.864723	1.289505
H	-2.131585	2.417662	0.000034	O	0.000008	-1.590616	0.000210
C	-0.000002	2.565204	0.000051	C	3.807373	0.623385	-0.000277
H	-0.000005	3.654006	0.000116	H	3.832303	1.268977	-0.887400
C	1.201859	1.851778	0.000033	H	3.832600	1.269068	0.886771
H	2.131582	2.417673	-0.000005	H	4.727410	0.022633	-0.000393
C	-2.580347	-0.309135	-0.000033	C	2.668514	-1.204149	-1.260723
C	-3.807362	0.623394	-0.000205	H	2.677770	-0.587177	-2.169334
H	-3.832567	1.268693	-0.887531	H	3.589694	-1.807502	-1.251218
H	-4.727406	0.022651	0.000160	H	1.799505	-1.864708	-1.289342
H	-3.832304	1.269370	0.886640	C	2.668815	-1.203913	1.260795
C	-2.668588	-1.204111	-1.260747	H	2.678247	-0.586779	2.169294
H	-2.677805	-0.587119	-2.169346	H	1.799829	-1.864489	1.289730
H	-1.799633	-1.864740	-1.289379	H	3.590012	-1.807240	1.251204

Table A1.5 (Continued).



Atom	X	Y	Z	Atom	X	Y	Z
Li	-0.125337	0.042745	-0.039737	H	-3.976780	-0.861579	-0.380558
O	2.179459	-0.262614	0.727516	H	-3.115961	-0.075254	0.969027
C	2.860212	-0.269250	-0.529438	H	-2.280537	-2.633217	-0.521633
C	2.234468	-1.276898	-1.477107	H	-2.933550	-2.539101	1.133467
O	0.862027	-0.923565	-1.654213	C	-0.342451	-2.964434	1.216323
C	0.186689	-1.771677	-2.582846	H	-0.887371	-3.508600	1.998685
H	0.217591	-2.819117	-2.252420	H	-0.235086	-3.616159	0.338469
H	-0.847654	-1.429629	-2.625929	H	0.643826	-2.687901	1.587461
H	0.645069	-1.699918	-3.577662	O	0.480389	1.978431	-0.755487
H	2.304910	-2.298297	-1.073272	C	0.176309	3.018555	0.171671
H	2.758263	-1.256745	-2.444292	C	0.293042	2.452503	1.570773
H	3.926666	-0.491477	-0.397471	O	-0.512648	1.275952	1.649314
H	2.764842	0.737682	-0.943257	C	-0.609676	0.776853	2.983835
C	2.846288	-1.004888	1.745565	H	0.387186	0.595932	3.408142
H	2.221346	-0.955226	2.639720	H	-1.145667	1.489723	3.623136
H	2.987253	-2.057427	1.463143	H	-1.158972	-0.162814	2.931074
H	3.826546	-0.565002	1.970343	H	1.336387	2.193704	1.796149
O	-1.020854	-1.757358	0.875443	H	-0.051756	3.202470	2.296522
C	-2.335302	-2.006175	0.380178	H	0.882456	3.853447	0.058840
C	-2.986415	-0.680012	0.060358	H	-0.838670	3.398211	-0.015752
O	-2.150514	0.014659	-0.864280	C	0.640568	2.448856	-2.092070
C	-2.791408	1.171603	-1.401567	H	1.503900	3.123284	-2.164520
H	-3.038721	1.890761	-0.609475	H	0.804825	1.569293	-2.715599
H	-2.095998	1.625714	-2.107152	H	-0.254294	2.984864	-2.435917
H	-3.710836	0.889883	-1.930447				

Table A1.5 (Continued).

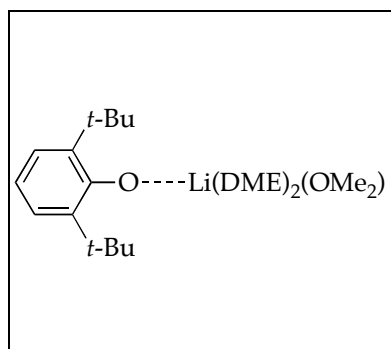
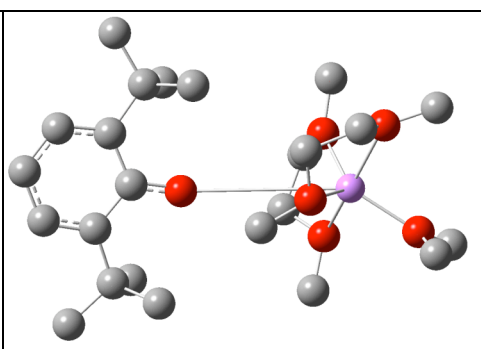


Atom	X	Y	Z	Atom	X	Y	Z
Li	2.288924	-0.056393	0.328573	H	0.141291	-1.751916	2.038305
O	3.956190	-1.308135	0.754839	H	-0.472963	-0.562858	3.211541
C	4.888699	-1.925650	-0.129681	O	1.447783	-1.490807	-0.937720
C	4.814663	-1.276056	-1.504021	C	0.458322	-0.854485	-1.776403
O	5.303394	0.057848	-1.537285	C	1.068534	0.431464	-2.287072
C	6.709075	0.152382	-1.695633	O	1.612883	1.143807	-1.172032
H	6.952537	1.216370	-1.745343	C	1.998416	2.472877	-1.509231
H	7.259874	-0.295795	-0.855158	H	2.762101	2.468491	-2.299696
H	7.037337	-0.332984	-2.627101	H	1.126797	3.047660	-1.845829
H	5.366330	-1.904791	-2.220708	H	2.409352	2.919571	-0.604585
H	3.767809	-1.238063	-1.816859	H	1.873165	0.242861	-3.015317
H	5.901512	-1.843119	0.293480	H	0.286098	1.029563	-2.771013
H	4.654417	-2.997867	-0.224642	H	0.227601	-1.507209	-2.631083
C	4.037800	-1.824384	2.080422	H	-0.463453	-0.665265	-1.208267
H	5.019386	-1.606958	2.524855	C	1.076161	-2.820229	-0.584050
H	3.249701	-1.339222	2.657404	H	1.078385	-3.468770	-1.471203
H	3.879721	-2.912305	2.087585	H	1.819993	-3.182169	0.130303
O	1.202591	-0.013611	2.097403	H	0.079043	-2.846325	-0.130705
C	1.133668	1.354219	2.500683	O	-2.156028	-0.192782	-0.275912
C	2.554972	1.867402	2.601144	C	-3.426902	0.048462	-0.092748
O	3.196279	1.612441	1.356070	C	-4.378049	-1.025175	0.124060
C	4.580074	1.940126	1.350236	C	-3.930905	-2.498677	-0.001534
H	4.724783	3.021396	1.483522	C	-5.083326	-3.500417	0.216475
H	5.110720	1.408908	2.153491	H	-5.510452	-3.425133	1.223623
H	4.972140	1.621695	0.383958	H	-5.894093	-3.359507	-0.507504
H	3.095679	1.347686	3.407086	H	-4.705318	-4.523886	0.094026
H	2.554641	2.944799	2.824936	C	-2.838331	-2.827055	1.041509
H	0.644776	1.437013	3.481910	H	-3.221571	-2.690904	2.060955
H	0.549165	1.933036	1.775351	H	-2.502387	-3.870506	0.943890
C	-0.068396	-0.693539	2.199864	H	-1.994665	-2.153331	0.893056
H	-0.786199	-0.337564	1.447954	C	-3.372207	-2.744661	-1.424256

Table A1.5 (Continued).

Atom	X	Y	Z
H	-4.163685	-2.617793	-2.172907
H	-2.576648	-2.028808	-1.638870
H	-2.978140	-3.767436	-1.520566
C	-5.709190	-0.716581	0.413738
C	-6.176060	0.595447	0.469187
C	-5.290590	1.632580	0.183904
C	-3.945049	1.402808	-0.113250
C	-3.022290	2.578305	-0.502921
C	-3.745850	3.939948	-0.503624
H	-4.128653	4.202802	0.489744
H	-3.043794	4.728022	-0.806411
H	-4.586558	3.958101	-1.206476
C	-1.835716	2.690409	0.482312
H	-2.197898	2.869216	1.503034
H	-1.273636	1.755731	0.464404
H	-1.176059	3.527727	0.205490
C	-2.478052	2.343404	-1.933018
H	-3.294641	2.371877	-2.664573
H	-1.750787	3.122358	-2.210886
H	-2.000974	1.362318	-1.984051
H	-5.674595	2.648452	0.190699
H	-7.217091	0.803872	0.704454
H	-6.418436	-1.517505	0.599508

Table A1.5 (Continued).

		<p>S35 G = -1401.074951 (-90 °C) see pg S102</p>
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Atom	X	Y	Z	Atom	X	Y	Z
Li	-2.757092	-0.217902	0.094217	C	-2.217857	2.310348	1.923897
O	-4.454943	-1.378406	-0.090207	H	-2.860418	2.373394	2.814684
C	-5.150116	-1.952763	1.010227	H	-1.271123	2.825857	2.123277
H	-4.600099	-1.681690	1.912373	H	-2.718365	2.773967	1.074422
H	-6.178905	-1.569993	1.066946	H	-2.063527	0.033794	3.419725
H	-5.181902	-3.047589	0.923073	H	-0.493139	0.789827	3.017962
C	-5.012586	-1.736715	-1.348369	H	-0.517329	-1.752127	2.846960
H	-6.036320	-1.349392	-1.452355	H	0.060986	-0.891198	1.382100
H	-4.369375	-1.302408	-2.114923	C	-1.580422	-2.997526	0.850797
H	-5.034180	-2.829099	-1.466998	H	-1.520128	-3.670848	1.717003
O	-1.925184	-0.121408	-1.775978	H	-2.394271	-3.320237	0.197078
C	-1.932445	1.236853	-2.214154	H	-0.628704	-3.033584	0.308362
C	-3.355705	1.743814	-2.123478	O	1.602165	-0.187683	0.333357
O	-3.804708	1.556524	-0.783915	C	2.819920	0.093101	-0.047948
C	-5.159956	1.932053	-0.591187	C	3.765259	-0.948434	-0.401244
H	-5.307748	2.997995	-0.813673	C	3.413245	-2.433629	-0.162570
H	-5.831164	1.339493	-1.228964	C	4.556471	-3.393225	-0.549593
H	-5.400562	1.745770	0.457413	H	4.798027	-3.337513	-1.617889
H	-4.008158	1.186496	-2.813294	H	5.472643	-3.189499	0.016349
H	-3.393669	2.808913	-2.397108	H	4.256057	-4.426595	-0.332958
H	-1.591947	1.299331	-3.257873	C	2.173108	-2.845482	-0.988723
H	-1.256326	1.838954	-1.595347	H	2.362165	-2.717989	-2.062514
C	-0.652022	-0.770200	-2.000125	H	1.918675	-3.901756	-0.814252
H	0.122213	-0.390854	-1.318977	H	1.332582	-2.212617	-0.704400
H	-0.817743	-1.832642	-1.816844	C	3.120092	-2.650431	1.342250
H	-0.350670	-0.633321	-3.046173	H	4.023079	-2.467233	1.937223
O	-1.884639	-1.670536	1.271637	H	2.342942	-1.959121	1.674188
C	-0.808115	-1.077429	2.028468	H	2.793394	-3.683163	1.535044
C	-1.334665	0.214028	2.613779	C	5.014833	-0.595634	-0.916739
O	-1.977228	0.952554	1.567999	C	5.411638	0.731861	-1.068192

Table A1.5 (Continued).

Atom	X	Y	Z
C	4.548747	1.740083	-0.643606
C	3.283423	1.465036	-0.119475
C	2.397541	2.608512	0.420122
C	3.067072	3.993436	0.312601
H	3.272650	4.272209	-0.727893
H	2.399974	4.757226	0.733569
H	4.011144	4.036866	0.867468
C	1.064770	2.680547	-0.360920
H	1.254455	2.868496	-1.425920
H	0.542804	1.728124	-0.254013
H	0.431870	3.498115	0.018589
C	2.097623	2.355104	1.917876
H	3.020900	2.403473	2.507624
H	1.406543	3.114950	2.315266
H	1.659985	1.361623	2.039108
H	4.887450	2.768939	-0.723385
H	6.388250	0.974853	-1.480106
H	5.715446	-1.372712	-1.207906

REFERENCES

1. (a) Green, J. R. In *Science of Synthesis*; Georg Thieme Verlag: New York, 2005; Vol. 8a, pp 427-486. (b) Schetter, B.; Mahrwald, R. *Angew. Chem., Int. Ed.* **2006**, *45*, 7506. (c) Arya, P.; Qin, H. *Tetrahedron* **2000**, *56*, 917. (d) Caine, D. In *Comprehensive Organic Synthesis*; Trost, B. M.; Fleming, I., Eds.; Pergamon: New York, **1989**, Vol. 1, p 1. Martin, S. F. *Ibid.*, Vol. 1, pg. 475. (e) Plaquevent, J.-C.; Cahard, D.; Guillen, F.; Green, J. R. In *Science of Synthesis*; Georg Thieme Verlag: New York, 2005; Vol. 26, pp 463-511. (f) *Comprehensive Organic Functional Group Transformations II*; Katritzky, Alan R.; Taylor, Richard J. K., Eds.; Elsevier: Oxford, UK, 1995, pp. 834-835. (g) Cativiela, C.; Diaz-de-Villegas, M. D. *Tetrahedron: Asymmetry* **2007**, *18*, 569.

2. (a) Jackman, L. M.; Bortiatynski, J. *Adv. Carbanion Chem.* **1992**, *1*, 45. (b) Zune, C.; Jerome, R. *Prog. Polymer Sci.* **1999**, *24*, 631. (c) Baskaran, D. *Prog. Polym. Sci.* **2003**, *28*, 521. (d) Suzuki, M.; Koyama, H.; Noyori, R. *Bull. Chem. Soc. Jpn.* **2004**, *77*, 259. (e) Suzuki, M.; Koyama, H.; Noyori, R. *Tetrahedron* **2004**, *60*, 1571. (f) Biddle, M. M.; Reich, H. J. *J. Org. Chem.* **2006**, *71*, 4031.

3. (a) Streitwieser, A.; Wang, D. Z. *J. Am. Chem. Soc.* **1999**, *121*, 6213. (b) Leung, S. S.-W.; Streitwieser, A. *J. Org. Chem.* **1999**, *64*, 3390. (c) Wang, D. Z.; Kim, Y.-J.; Streitwieser, A. *J. Am. Chem. Soc.* **2000**, *122*, 10754. (d) Kim, Y.-J.; Streitwieser, A. *Org. Lett.* **2002**, *4*, 573. (e) Kim, Y.-J.; Wang, D. Z. *Org. Lett.* **2001**, *3*, 2599. (f) Streitwieser, A.; Leung, S. S.-W.; Kim, Y.-J. *Org. Lett.* **1999**, *1*, 145. (g) Abboto, A.; Leung, S. S.-W.; Streitwieser, A.; Kilway, K. V. *J. Am. Chem. Soc.* **1998**, *120*, 10807. (h) Leung, S. S.-W.; Streitwieser, A. *J. Am. Chem. Soc.* **1998**, *120*, 10557. (i) Abu-

Hasanayn, F.; Streitwieser, A. *J. Org. Chem.* **1998**, *63*, 2954. (j) Abu-Hasanayn, F.; Streitwieser, A. *J. Am. Chem. Soc.* **1996**, *118*, 8136. (k) Gareyev, R.; Ciula, J. C.; Streitwieser, A. *J. Org. Chem.* **1996**, *61*, 4589. (l) Abu-Hasanayn, F.; Stratakis, M.; Streitwieser, A. *J. Org. Chem.* **1995**, *60*, 4688. (m) Dixon, R. E.; Williams, P. G.; Saljoughian, M.; Long, M. A.; Streitwieser, A. *Magn. Reson. Chem.* **1991**, *29*, 509.

4. (a) Arnett, E. M.; Moe, K. D. *J. Am. Chem. Soc.* **1991**, *113*, 7288. (b) Arnett, E. M.; Fisher, F. J.; Nichols, M. A.; Ribeiro, A. A. *J. Am. Chem. Soc.* **1990**, *112*, 801. (c) Seebach, D.; Bauer, von W. *Helv. Chim. Acta* **1984**, *67*, 1972. (d) Shobatake, K.; Nakamoto, K. *Inorg. Chim. Acta* **1980**, *4*, 485. (e) den Besten, R.; Harder, S.; Brandsma, L. *J. Organomet. Chem.* **1990**, *385*, 153. (f) Halaska, V.; Lochmann, L. *Collect. Czech. Chem. Commun.* **1973**, *38*, 1780. (g) Golovanov, I. B.; Simonov, A. P.; Priskunov, A. K.; Talalseva, T. V.; Tsareva, G. V.; Kocheshkov, *Dokl. Akad. Nauk. SSSR* **1963**, *149*, 835. (h) Simonov, A. P.; Shigorin, D. N.; Talalseva, T. V.; Kocheshkov, K. A. *Bull. Acad. Sci. USSR Div. Chem. Sci.* **1962**, *6*, 1056. (i) Armstrong, D. R.; Davies, J. E.; Davies, R. P.; Raithby, P. R.; Snaith, R.; Wheatley, A. E. H. *New J. Chem.* **1999**, 35. (j) Nichols, M. A.; Leposa, C. *Abstracts of Papers*, 38th Central Regional Meeting of the American Chemical Society, Frankenmuth, MI, May 16-20, 2006; American Chemical Society: Washington, D. C. (k) Lochmann, L.; Lim, D. *J. Organomet. Chem.* **1973**, *50*, 9.

5. (a) Jackman, L. M.; Lange, B. C. *Tetrahedron* **1977**, *33*, 2737. (b) Jackman, L. M.; DeBrosse, C. W. *J. Am. Chem. Soc.* **1983**, *105*, 4177. (c) Jackman, L. M.; Smith, B. D. *J. Am. Chem. Soc.* **1988**, *110*, 3829. (d) Jackman, L. M.; Chen, X. *J. Am. Chem. Soc.* **1992**, *114*, 403. (e) Jackman, L. M.; Rakiewicz, E. F.; Benesi, A. J. *J. Am. Chem. Soc.* **1991**, *113*, 4101. (f) Also, see ref 4a.

6. (a) McNeil, A. J.; Toombes, G. E. S.; Chandramouli, S. V.; Vanasse, B. J.; Ayers, T. A.; O'Brien, M. K.; Lobkovsky, E.; Gruner, S. M.; Marohn, J. A.; Collum, D. B. *J. Am. Chem. Soc.* **2004**, *126*, 5938. (b) McNeil, A. J.; Toombes, G. E. S.; Gruner, S. M.; Lobkovsky, E.; Collum, D. B.; Chandramouli, S. V.; Vanasse, B. J.; Ayers, T. A. *J. Am. Chem. Soc.* **2004**, *126*, 16559. (c) McNeil, A. J.; Collum, D. B. *J. Am. Chem. Soc.* **2005**, *127*, 5655. (d) Liou, L. R.; McNeil, A. J.; Toombes, G. E. S.; Collum, D. B., *J. Am. Chem. Soc.* **2008**, *130*, 17334.
7. (a) Liou, L. R.; McNeil, A. J.; Ramirez, A.; Toombes, G. E. S.; Gruver, J. M.; Collum, D. B. *J. Am. Chem. Soc.* **2008**, *130*, 4859. (b) Gruver, J. M.; Liou, L. R.; McNeil, A. J.; Ramirez, A.; Collum, D. B. *J. Org. Chem.* **2008**, *73*, 7743.
8. Günther, H. *J. Braz. Chem. Soc.* **1999**, *10*, 241.
9. (a) Collum, D. B. *Acc. Chem. Res.* **1993**, *26*, 227. (b) Lucht, B. L.; Collum, D. B. *Acc. Chem. Res.* **1999**, *32*, 1035.
10. Job, P. *Ann. Chim.* **1928**, *9*, 113.
11. (a) Gil, V. M. S.; Oliveira, N. C. *J. Chem. Educ.* **1990**, *67*, 473. (b) Huang, C. Y. *Method Enzymol.* **1982**, *87*, 509. (c) Hirose, K. *J. Incl. Phenom.* **2001**, *39*, 193. (d) Likussar, W.; Boltz, D. F. *Anal. Chem.* **1971**, *43*, 1265.
12. Goralski, P.; Legoff, D.; Chabanel, M. *J. Organomet. Chem.* **1993**, *456*, 1.

13. Kissling R. M.; Gagne, M. R. *J. Org. Chem.* **2001**, *66*, 9005.
14. (a) Günther, H. In *Advanced Applications of NMR to Organometallic Chemistry*; Gielen, M., Willem, R., Wrackmeyer, B., Eds.; Wiley & Sons: New York, 1996; pp 247-290. (b) Eppers, O.; Günther, H. *Helv. Chem. Acta* **1992**, *75*, 2553. (c) Eppers, O.; Günther, H. *Helv. Chim. Acta* **1990**, *73*, 2071. (d) Also see ref 8.
15. (a) Novak, D. P.; Brown, T. L. *J. Am. Chem. Soc.* **1972**, *94*, 3793. (b) Desjardins, S.; Flinois, K.; Oulyadi, H.; Davoust, D.; Giessner-Prettre, C.; Parisel, O.; Maddaluno, J. *Organometallics* **2003**, *22*, 4090. (c) Seitz, L. M.; Brown, T. L. *J. Am. Chem. Soc.* **1966**, *88*, 2174. (d) Weiner, M. A.; West, R. *J. Am. Chem. Soc.*, **1963**, *85*, 485. (e) Maddaluno, J. *Organometallics* **2008**, *27*, 3564. (f) Pospisil, P. J.; Wilson, S. R.; Jacobsen, E. N. *J. Am. Chem. Soc.* **1992**, *114*, 7585. (g) See ref 2f.
16. Dugger, R. W.; Ragan, J. A.; Ripin, D. H. B. *Org. Process Res. Dev.* **2005**, *9*, 253.
17. For reviews of organolithium chemistry in pharmaceutical process research, see: (a) Farina, V.; Reeves, J. T.; Senanayake, C. H. Song, J. J. *Chem. Rev.* **2006**, *106*, 2734. (b) Wu, G.; Huang, M. *Chem. Rev.* **2006**, *106*, 2596. (c) Rathman, T. L.; Bailey, W. F. *Org. Process Res. Dev.* **2009**, *13*, 144.
18. Lithium phenolates are useful in organometallic synthesis: Cetinkaya, B.; Gümrükcü, I.; Lappert, M. F.; Atwood, J. L.; Shakir, R. *J. Am. Chem. Soc.* **1980**, *102*, 2086.

19. "Pharmaceuticals & Intermediates 1986-1997 Update"; Becker, A., Ed.; Becker Associates, 1997.

20. Studies of lithium phenolate reactivity: (a) Jackman, L. M.; Chen, X. *J. Am. Chem. Soc.* **1997**, *119*, 8681. (b) Jackman, L. M.; Petrei, M. M.; Smith, B. D. *J. Am. Chem. Soc.* **1991**, *113*, 3451. (c) See ref 2a.

21. A number of phenolates in Table 1 have been characterized crystallographically. The coordinating solvent and resulting aggregation states are as follows: (a) **7** (THF), hexamer: Jackman, L. M.; Çizmeciyen, D.; Williard, P. G.; Nichols, M. A. *J. Am. Chem. Soc.* **1993**, *115*, 6262. (b) **7** (THF), tetramer: Boyle, T. J.; Pedrotty, D. M.; Alam, T. M.; Vick, S. C.; Rodriguez, M. A. *Inorg. Chem.* **2000**, *39*, 5133. (c) **13** (THF), tetramer: Rosen, T. C.; Kirschbaum, K.; Giolando, D. M. *Inorg. Chim. Acta* **2005**, *358*, 3680. (d) **21** (THF), tetramer: see ref. 21b. (e) **24** (THF), dimer: see ref 21b. (f) **25** (THF), tetramer: see ref 21b. (g) **27** (THF), trimer: see ref 21b. (h) **30** (THF), dimer: Huffman, J. C.; Geerts, R. L.; Caulton, K. G. *J. Crystallogr. Spectrosc. Res.* **1984**, *14*, 541; see also ref 21b. (i) **32** (THF), dimer: Clegg, W.; Lamb, E.; Liddle, S. T.; Snaith, R.; Wheatley, A. E. H. *J. Organomet. Chem.* **1999**, *573*, 305.

22. Jackman observed a putative hexamer in more poorly coordinating solvents (ref 5). b-amino ester enolates are uniformly hexameric in THF (ref 6).

23. For a discussion of crystallographic studies of lithium phenolates, see: Cole, M. L.; Junk, P. C.; Proctor, K. M.; Scott, J. L.; Strauss, C. R. *Dalton Trans.* **2006**, 3338.

24. After surveying a subset of the community, we have chosen to refer to $(\text{LiX})_n$ and $(\text{LiX})_m(\text{LiX}')_n$ as a “homoaggregate” and “heteroaggregate”, respectively, and reserve the term “mixed aggregate” for $(\text{LiX})_m(\text{LiY})_n$.
25. (a) Brown, T. L. *Acc. Chem. Res.* **1968**, *1*, 23.
26. Trimeric lithium phenolates have occasionally been observed in the solid state bearing pendant amine ligands. See, for example: van der Schaaf, P. A.; Jastrzebski, J. T. B. H.; Hogerheide, M. P.; Smeets, W. J. J.; Spek, A. L.; Boersma, J.; van Koten, G. *Inorg. Chem.* **1993**, *32*, 4111. Also, see ref 21g.
27. Mulvey, R. E. *Chem. Soc. Rev.* **1991**, *20*, 167. Also, see ref 29.
28. (a) Arvidsson, P. I.; Ahlberg, P.; Hilmersson, G. *Chem. Eur. J.* **1999**, *5*, 1348. (b) Bauer, W. *J. Am. Chem. Soc.* **1996**, *118*, 5450. (c) Bauer, W.; Griesinger, C. *J. Am. Chem. Soc.* **1993**, *115*, 10871. (d) DeLong, G. T.; Pannell, D. K.; Clarke, M. T.; Thomas, R. D. *J. Am. Chem. Soc.* **1993**, *115*, 7013. (e) Thomas, R. D.; Clarke, M. T.; Jensen, R. M.; Young, T. C. *Organometallics* **1986**, *5*, 1851. (f) Bates, T. F.; Clarke, M. T.; Thomas, R. D. *J. Am. Chem. Soc.* **1988**, *110*, 5109. (g) Fraenkel, G.; Hsu, H.; Su, B. M. In *Lithium: Current Applications in Science, Medicine, and Technology*; Bach, R. O., Ed.; Wiley: New York, 1985; pp 273-289. (h) Heinzer, J.; Oth, J. F. M.; Seebach, D. *Helv. Chim. Acta* **1985**, *68*, 1848. (i) Fraenkel, G.; Henrichs, M.; Hewitt, J. M.; Su, B. M.; Geckle, M. J. *J. Am. Chem. Soc.* **1980**, *102*, 3345. (j) Lucht, B. L.; Collum, D. B. *J. Am. Chem. Soc.* **1996**, *118*, 3529. (k) Knorr, R.; Menke, T.; Ferchland, K.; Mahlstäubl, J.; Stephenson, D. S. *J. Am. Chem. Soc.* **2008**, *130*, 14179.

29. Although we cannot find evidence of five-rung (pentameric) ladders in the crystallographic literature, we observed them as part of nearly statistical ensembles of 3-, 4-, 5- and 6-rung lithium diethylamide ladders: Rutherford, J. L.; Collum, D. B. *J. Am. Chem. Soc.* **1999**, *121*, 10198.
30. (a) Williard, P. G.; Hintze, M. J. *J. Am. Chem. Soc.* **1990**, *112*, 8602. (b) Godenschwager, P. F.; Collum, D. B. *J. Am. Chem. Soc.* **2007**, *129*, 12023.
31. (a) [^6Li , ^{15}N] LiHMDs (ref 31b) allows us to detect mixed dimers. (b) Romesberg, F. E.; Bernstein, M. P.; Gilchrist, J. H.; Harrison, A. T.; Fuller, D. J.; Collum, D. B. *J. Am. Chem. Soc.* **1993**, *115*, 3475.
32. For early discussions of steric effects on solvation and aggregation, see: Settle, F. A.; Haggerty, M.; Eastham, J. F. *J. Am. Chem. Soc.* **1964**, *86*, 2076. Lewis, H. L.; Brown, T. L. *J. Am. Chem. Soc.* **1970**, *92*, 4664. Brown, T. L.; Gerteis, R. L.; Rafus, D. A.; Ladd, J. A. *J. Am. Chem. Soc.* **1964**, *86*, 2135. For a discussion and more recent leading references, see: Zhao, P.; Collum, D. B. *J. Am. Chem. Soc.* **2003**, *125*, 14411.
33. In previous manuscripts we examined the efficacy of parametric fits to distinguish the all-dimer $\text{A}_2\text{-AB-B}_2$ model from the $\text{A}_2\text{-AB-B}_4$ or $\text{A}_2\text{-AB-B}$ models as well as the all tetramer $\text{A}_4\text{-A}_3\text{B-A}_2\text{B}_2\text{-A}_1\text{B}_3\text{-B}_4$ model from the $\text{A}_4\text{-A}_3\text{B-A}_2\text{B}_2\text{-A}_1\text{B}_3\text{-B}_2$ model with one homodimer (ref 6 and 7). Focusing on the dimer-dominated example emblematically, $\text{A}_2\text{-AB-B}$ and $\text{A}_2\text{-AB-B}_4$ models become indistinguishable from $\text{A}_2\text{-AB-B}_2$ by parametric fit at very low or very high relative AB concentration. It is

ironic, therefore, that the parametric fits become less effective precisely when the deviation from statistical shows the distinction is most needed.

34. (a) Qu, B.; Collum, D. B. *J. Am. Chem. Soc.* **2006**, *128*, 9355. (b) Bernstein, M.P.; Romesberg, F. E.; Fuller, D. J.; Harrison, A. T.; Williard, P. G.; Liu, Q. Y.; Collum, D. B. *J. Am. Chem. Soc.* **1992**, *114*, 5100.

35. Standard ethereal ligands have been observed coordinated to lithium ion in the slow exchange limit only rarely and only at very low temperatures. Leading references: (a) Arvidsson, P. I.; Davidsson, Ö. *Angew. Chem., Int. Ed. Engl.* **2000**, *39*, 1467. (b) Sikorski, W. H.; Reich, H. J. *J. Am. Chem. Soc.* **2001**, *123*, 6527. (c) Leading references in ref 7.

36. (a) One can infer approximate relative solvent binding constants from the proportions of the two solvents required to achieve a 50% shift. In Figure 9c, for example, the average chemical shift at equimolar THF and DME suggests a preference for the THF-solvated dimer. (b) If two different aggregation states are observed from a solvent swap, one can extract a relative binding constants as well: Remenar, J. F.; Lucht, B. L.; Collum, D. B. *J. Am. Chem. Soc.* **1997**, *119*, 5567.

37. Our first experience with solvent swaps occurred during studies of unsolvated lithium diisopropylamide in which addition of a weakly coordinating trialkylamine caused only one of several unsolvated cyclic oligomers to migrate to the chemical shift of the disolvated dimer (ref 34b).

38. The crystal structure of a mixed dimer of **30** with Me₂AlOAr is unsolvated at Li with stabilizing Li⁺⋯H(*t*-Bu)agostic interactions (ref 21i)
39. The temperature-dependent change in solvation with warming is inferred to be desolvation because of the substantial negative enthalpies of solvation. For related desolvations, see ref 34 and 53.
40. (a) Kremer, T.; Schleyer, P. v. R. *Organometallics* **1997**, *16*, 737. (b) MacDougall, D. J.; Noll, B. C.; Kennedy, A. R.; Henderson, K. W. *J. Chem. Soc., Dalton Trans.* **2006**, 1875. (c) Strohmman, C.; Dilsky, F.; Strohfeltdt, K. *Organometallics* **2006**, *25*, 41.
41. For leading references to theoretical studies of O-lithiated species, see: (a) Khartabi, H. K.; Gros, P. C.; Fort, Y.; Ruiz-Lopez, M. F. *J. Org. Chem.* **2006**, *73*, 9393. (b) Streitwieser, A. *J. Mol. Model.* **2006**, *12*, 673. (c) Pratt, L. M.; Streitwieser, A. *J. Org. Chem.* **2003**, *68*, 2830. (d) Pratt, L. M.; Nguyen, S. C.; Thanh, B. T. *J. Org. Chem.* **2008**, *73*, 6086.
42. *Gaussian 03*, revision B.04; Gaussian, Inc.: Pittsburgh, PA, 2003. See Supporting Information for the full list of authors.
43. Rutherford, J. L.; Hoffmann, D.; Collum, D. B. *J. Am. Chem. Soc.* **2002**, *124*, 264.
44. Leading references to salt effects: (a) Tchoubar, B.; Loupy, A. *Salt Effects in Organic and Organometallic Chemistry*; VCH: New York, 1992; Chapters 4, 5, and 7. (b) Seebach, D. In *Proceedings of the Robert A. Welch Foundation Conferences on*

- Chemistry and Biochemistry*; Wiley: New York, 1984; p 93. (c) Gossage, R. A.; Jastrzebski, J. T. B. H.; van Koten, G. *Angew. Chem., Int. Ed.* **2005**, *44*, 1448. (d) Seebach, D. *Angew. Chem., Int. Ed. Engl.* **1988**, *27*, 1624.
45. (a) Hsieh, H. L.; Quirk, R. P. *Anionic Polymerization: Principles and Practical Applications*; Marcel Dekker: New York, 1996. (b) *Ions and Ion Pairs in Organic Reactions*; Szwarc, M., Ed.; Wiley: New York, 1972; Vol. 1 and 2.
46. (a) Hassoun, J.; Reale, P.; Scrosati, B. *J. Materials Chem.* **2007**, *17*, 3668. (b) Lithium phenolate has been examined as an electrolyte for lithium batteries: Barthel, J.; Buestrich, R.; Gores, H. J.; Schmidt, M.; Wuhr, M. *J. Electrochem. Soc.* **1997**, *144*, 3866.
47. (a) Komoroski, R. A. *Magn. Reson Imag.* **2000**, *18*, 103. (b) Johnson, F. N. *Rev. Contemp. Pharmacotherapy* **1999**, *10*, 193.
48. Adhvaryu, A.; Sung, C.; Erhan, S. Z. *Indust. Crops. Prod.* **2005**, *21*, 285.
49. Burgess, J. *Metal Ions in Solution*, Wiley: New York, 1978. Goralski, P.; Chabanel, M. *Inorg. Chem.* **1987**, *26*, 2169 and references cited therein.
50. (a) Galiano-Roth, A. S.; Michaelides, E. M.; Collum, D. B. *J. Am. Chem. Soc.* **1988**, *110*, 2658. (b) Reich, H. J.; Goldenberg, W. S.; Gudmundsson, B. Ö.; Sanders, A. W.; Kulicke, K. J.; Simon, K.; Guzei, I. A. *J. Am. Chem. Soc.* **2001**, *123*, 8067. (c) Gilchrist, J. H.; Harrison, A. T.; Fuller, D. J.; Collum, D. B. *J. Am. Chem. Soc.* **1990**, *112*, 4069. (d) Hoffmann, D.; Collum, D. B. *J. Am. Chem. Soc.* **1998**, *120*, 5810. (e)

Jacobson, M. A.; Keresztes, I.; Williard, P. G. *J. Am. Chem. Soc.* **2005**, *127*, 4965. (g)
Reich, H. J.; Holladay, J. E. *J. Am. Chem. Soc.* **1995**, *117*, 8470. (h) Also, see ref 5d.

51. Diffusion-ordered NMR spectroscopy (DOSY) shows considerable potential to examine the structures of LiX salts: Li, D.; Keresztes, I.; Hopson, R.; Williard, P. G. *Acc. Chem. Res.* **2009**, *42*, 270.

52. Ramirez, A.; Sun, X.; Collum, D. B. *J. Am. Chem. Soc.* **2006**, *128*, 10326.

53. Lucht, B. L.; Collum, D. B. *J. Am. Chem. Soc.* **1995**, *117*, 9863.

54. (a) +Li(THF)₅: Olmstead, M. M.; Power, P. P.; Sigel, G. *Inorg. Chem.* **1986**, *25*, 1027. (b) +Li(THF)₆: Schenk, C.; Schnepf, A. *Angew. Chem., Int. Ed. Engl.* **2007**, *46*, 5314.

55. (a) Lucht, B. L.; Bernstein, M. P.; Remenar, J. F.; Collum, D. B. *J. Am. Chem. Soc.* **1996**, *118*, 10707. (b) Scheschkewitz, D. *Angew. Chem., Int. Ed. Engl.* **2004**, *43*, 2965. (c) Niecke, E.; Nieger, M.; Schmidt, O.; Gudat, D.; Schoeller, W. W. *J. Am. Chem. Soc.* **1999**, *121*, 519. (d) Becker, G.; Eschbach, B.; Mundt, O.; Reti, M.; Niecke, E.; Issberger, K.; Nieger, M.; Thelen, V.; Noth, H.; Waldhor, R.; Schmidt, M. *Z. Anorg. Allg. Chem.* **1998**, *624*, 469. (e) Rogers, R. D.; Bynum, R. V.; Atwood, J. L. *J. Crystallogr. Spectrosc. Res.* **1984**, *14*, 29. (f) Riffel, H.; Neumuller, B.; Fluck, E. *Z. Anorg. Allg. Chem.* **1993**, *619*, 1682. (g) Becker, G.; Schwarz, W.; Seidler, N.; Westerhausen, M. *Z. Anorg. Allg. Chem.* **1992**, *612*, 72. (h) Wang, H.; Wang, H.; Li, H.-W.; Xie, Z. *Organometallics* **2004**, *23*, 875. (i) Xu, X.; Zhang, Z.; Yao, Y.; Zhang, Y.; Shen, Q. *Inorg. Chem.* **2007**, *46*, 9379. (j) Xiang-Gao, L.; Jing-Zhi, L.;

Shong-Chen, J.; Yong-Hua, L.; Guo-Zhi, L. *Chin. J. Struct. Chem.* **1991**, *10*, 60. (k)
 Thiele, K.; Goris, H.; Imhof, W.; Seide, W. *Z. Anorg. Allg. Chem.* **2002**, 628, 107. (l)
 Ramirez, A.; Lobkovsky, E.; Collum, D. B. *J. Am. Chem. Soc.* **2003**, *125*, 15376.

56. LiX(DME)₂(THF): (a) Wang, H.; Wang, H.; Li, H.-W.; Xie, Z. *Organometallics* **2004**, *23*, 875. (b) Xu, X.; Zhang, Z.; Yao, Y.; Zhang, Y.; Shen, Q. *Inorg. Chem.* **2007**, *46*, 9379. (c) Xiang-Gao, L.; Jing-Zhi, L.; Shong-Chen, J.; Yong-Hua, L.; Guo-Zhi, L. *Chin. J. Struct. Chem.* **1991**, *10*, 60. (d) Thiele, K.; Goris, H.; Imhof, W.; Seide, W. *Z. Anorg. Allg. Chem.* **2002**, 628, 107.

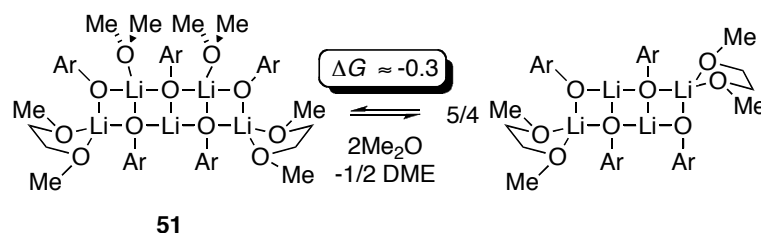
57. Recent representative examples: (a) Buchalski, P.; Grabowska, I.; Kaminska, E.; Suwinska, K. *Organometallics* **2008**, *27*, 2346. (b) Wang, Y.; Liu, D.; Chan, H.-S.; Xie, Z. *Organometallics* **2008**, *27*, 2825. (c) Braunschweig, H.; Burzler, M.; Dewhurst, R. D.; Radacki, K. *Angew. Chem., Int. Ed. Engl.* **2008**, *47*, 5650.

58. (a) Hilmersson, G.; Davidsson, O. *J. Org. Chem.* **1995**, *60*, 7660. (b) Williard, P. G.; Nichols, M. A. *J. Am. Chem. Soc.* **1993**, *115*, 1568. (c) Barnett, N. D. R.; Mulvey, R. E.; Clegg, W.; O'Neil, P. A. *J. Am. Chem. Soc.* **1993**, *115*, 1573. (d) Black, S. J.; Hibbs, D. E.; Hursthouse, M. B.; Jones, C.; Steed, J. W. *J. Chem. Soc., Chem. Commun.* **1998**, 2199. (e) Bruce, S.; Hibbs, D. E.; Jones, C.; Steed, J. W.; Thomas, R. C.; Williams, T. C. *New J. Chem.* **2003**, *27*, 466. (f) Hahn, F. E.; Keck, M.; Raymond, K. N. *Inorg. Chem.* **1995**, *34*, 1402. (g) Henderson, K. W.; Dorigo, A. E.; Liu, Q.-Y.; Williard, P. G. *J. Am. Chem. Soc.* **1997**, *119*, 11855. (h) Deacon, G. B.; Feng, T.; Hockless, D. C. R.; Junk, P. C. J.; Skelton, B. W.; Smith, M. K.; White, A. H. *Inorg. Chim. Acta* **2007**, *360*, 1364. (i) McGeary, M. J.; Coan, P. S.; Folting, K.; Streib, W. E.; Caulton, K. G. *Inorg. Chem.* **1991**, *30*, 1723. (j) Coan, P. S.; Streib, W. E.;

Caulton, K. G. *Inorg. Chem.* **1991**, *30*, 5019. (k) McGeary, M. J.; Cayton, R. H.; Folting, K.; Huffman, J. C.; Caulton, K. G. *Polyhedron* **1992**, *11*, 1369. (l) Bochkarev, M. N.; Fedushkin, I. L.; Fagin, A. A.; Petrovskaya, T. V.; Ziller, J. W.; Broomhall-Dillard, R. N. R.; Evans, W. J. *Angew. Chem., Int. Ed. Engl.* **1997**, *36*, 133. (m) Cosgriff, J. E.; Deacon, G. B.; Fallon, G. D.; Gatehouse, B. M.; Schumann, H.; Weimann, R. *Chem. Ber.* **1996**, *129* 953. (n) Deacon, G. B.; Delbridge, E. E.; Fallon, G. D.; Jones, C.; Hibbs, D. E.; Hursthouse, M. B.; Skelton, B. W.; White, A. H. *Organometallics* **2000**, *19*, 1713. (o) Link, H.; Fenske, D. Z. *Angew. Chem.* **1999**, *625*, 1878. (p) Bonomo, L.; Solari, E.; Scopelliti, R.; Latronico, M.; Floriani, C. J. *Chem. Soc., Chem. Commun.* **1999**, 2229. (q) Rosa, P.; Mezailles, N.; Ricard, L.; Le Floch, P. *Angew. Chem., Int. Ed. Engl.* **2000**, *39* 1823. (r) Iravani, E.; Neumuller, B. *Organometallics* **2005**, *24*, 842. (s) Lucht, B. L.; Bernstein, M. P.; Remenar, J. F.; Collum, D. B. *J. Am. Chem. Soc.* **1996**, *118*, 10707. (t) See ref 36.

59. The hindered chelating ligand, TMEDA, affords no cyclic trimers (ref 7b).

60. Tetrameric ladders are suggested to be of nearly equal stability when compared with the corresponding pentamers:



*Both U-shaped; energy in kcal/mol on a per-lithium basis at -90 °C.

61. The tendency for electron-withdrawing groups to promote deaggregation was noted by spectroscopic studies of Jackman and coworkers (ref 5) and has previously been suggested based on combination of computations and crystal structures Henderson and coworkers (ref 40b).

62. Bordwell, F. G.; McCallum, R. J.; Olmstead, W. N. *J. Org. Chem.*, **1984**, 49 (8), 1424.

63. (a) Stanciu, C.; Olmstead, M. M.; Phillips, A. D.; Stender, M.; Power, P. P. *Eur. J. Inorg. Chem.*, **2003**, 3495; and unsolvated trimers: (b) Vilardo, J. S.; Fanwick, P. E.; Rothwell, I. P. *Polyhedron* **1998**, 17, 769.

64. Yang, H.; Hay, A. S. *Synthesis* **1992**, 467.